Supplementary information for:

C C(sp^3)–H Cyclizations of 2-(2-Vinyl)phenoxy-*tert*-anilines

Petra Dunkel,[*,a] Dóra Bogdán,[a] Ruth Deme,[a] Ádám Zimber,[a] Veronika Ballayová,[a,b] Eszter Csizmadia,[a] Bence Kontra,[a,c] Eszter Kalydi,[a] Attila Bényei,[d] Péter Mátyus,[a,e] Zoltán Mucsi,[*,c,f,g]

[a]*Department of Organic Chemistry, Semmelweis University, Hőgyes Endre utca 7, H-1092 Budapest, Hungary, E-mail: dunkel.petra@semmelweis.hu*

[b]*Department of Chemical Drugs, Masaryk University, Palackého 1946/1, 612 00 Brno, Czech Republic*

[c]*Brain Vision Center, Department of Biological Chemistry, Liliom utca 43-45, H-1094 Budapest, Hungary*

[d]*Institute of Physical Chemistry, University of Debrecen, Egyetem tér 1, H-4010 Debrecen, Hungary*

[e]*University of Veterinary Medicine, István utca 2, H-1078 Budapest, Hungary*

[f]*Department of Chemistry, Femtonics Ltd., Tűzoltó utca 59, H-1094 Budapest, Hungary, E-mail: zmucsi@femtonics.eu*

[g]*Institute of Chemistry, University of Miskolc, Egyetem út 1, H-3515 Miskolc, Hungary*

Table of contents

Table S3. Computed energies (E), zero point energies, internal energies (U), enthalpies (H) and Gibbs free energies (G) given in Hartree as well as entropies (S) given in J mol^{-1} K^{-1} at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of the solvent applied.

			E	ZPE	U	H	G	S
0001aaa_pentadiene_B3LYP631dp_PCMw.log			-195.31790169	-195.204286	-195.198288	-195.197343	-195.233247	75.566
0001aba_pentadiene_B3LYP631dp_PCMdmso.log			-195.31787355	-195.204256	-195.198257	-195.197313	-195.233216	75.565
0001aca_pentadiene_B3LYP631dp_PCMmecn.log			-195.31785205	-195.204233	-195.198234	-195.197290	-195.233193	75.565
0001ada_pentadiene_B3LYP631dp_PCMdce.log			-195.31763906	-195.204001	-195.198004	-195.197060	-195.232959	75.556
0001aea_pentadiene_B3LYP631dp_PCMtol.log			-195.31692093	-195.203230	-195.197233	-195.196289	-195.232186	75.551
0001afa_pentadiene_B3LYP631dp_vacuo.log			-195.31617216	-195.202406	-195.196416	-195.195472	-195.231343	75.496
0001baa_pentadiene_TS_b3lyp631dp_PCMw.log			-195.26309710	-195.153001	-195.148362	-195.147418	-195.180289	69.183
0001bba_pentadiene_TS_b3lyp631dp_PCMdmso.log			-195.26306995	-195.152969	-195.148330	-195.147386	-195.180257	69.183
0001bca_pentadiene_TS_b3lyp631dp_PCMacn.log			-195.26304869	-195.152947	-195.148308	-195.147364	-195.180235	69.182
0001bda_pentadiene_TS_b3lyp631dp_PCMdce.log			-195.26283924	-195.152712	-195.148075	-195.147131	-195.179999	69.176
0001bea_pentadiene_TS_b3lyp631dp_PCMtol.log			-195.26212752	-195.151922	-195.147290	-195.146346	-195.179205	69.158
0001bfa_pentadiene_TS_b3lyp631dp_vacuo.log			-195.26137793	-195.151106	-195.146478	-195.145534	-195.178386	69.143

Table S4. Computed energies (E), zero point energies, internal energies (U), enthalpies (H) and Gibbs free energies (G) given in Hartree as well as entropies (S) given in J mol^{-1} K^{-1} at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of the solvent applied.

			E	ZPE	U	H	G	S
0101aaa_Ph_NMeBn_CHC_H_CN_B3lyp631pd_PCMdmso.log			-766.94380112	-766.656461	-766.639753	-766.638809	-766.702420	133.880
0101aaa_Ph_NMeBn_CHC_H_CN_ZW_INT_B3lyp631pd_PCMdmso.log			-766.87829798	-766.592692	-766.575822	-766.574878	-766.639173	135.321
0101daa_Ph_NMeBn_CHC_H_CN_ZW_INT_B3lyp631pd_PCMdmso_TS_CH.log			-766.87756629	-766.593863	-766.577668	-766.576724	-766.638829	130.712
0108aaa_Ph_NMeBn_CHC_H_CN_product_B3lyp631pd_PCMdmso.log			-766.95996671	-766.670420	-766.654675	-766.653731	-766.713986	126.817
0108baa_Ph_NMeBn_CHC_H_CN_product_B3lyp631pd_PCMdmso.log			-766.95785697	-766.668347	-766.652475	-766.651531	-766.712671	128.681
0201aaa_Ph_NMeBn_CHC_Me_COOMe_B3lyp631pd_PCMdmso.log			-941.89828990	-941.538889	-941.517871	-941.516927	-941.591132	156.178
0202aaa_Ph_NMeBn_CHC_Me_COOMe_ZW_INT_B3lyp631pd_PCMdmso.log			-941.83182498	-941.474415	-941.453282	-941.452338	-941.526596	156.290
0203daa_Ph_NMeBn_CHC_Me_COOMe_ZW_INT_B3lyp631pd_PCMdmso_TS_CH.log			-941.83102850	-941.474196	-941.453727	-941.452783	-941.525090	152.183
0208aba_Ph_NMeBn_CHC_Me_COOMe_product_B3lyp631pd_PCMdmso.log			-941.91538054	-941.553707	-941.533781	-941.532836	-941.602166	145.916
0208abb_Ph_NMeBn_CHC_Me_COOMe_product_B3lyp631pd_PCMdmso.log			-941.91232294	-941.550880	-941.530986	-941.530042	-941.599543	146.278
0301aaa_Ph_NMeBn_CHC_COOMe_CN_B3lyp631pd_PCMdmso.log			-994.82314482	-994.492838	-994.471622	-994.470678	-994.545227	156.903
0301daa_Ph_NMeBn_CHC_COOMe_CN_ZW_INT_B3lyp631pd_PCMdmso_TS_CH.log			-994.77751645	-994.451732	-994.430970	-994.430026	-994.503460	154.556
0308aaa_Ph_NMeBn_CHC_COOMe_CN_product_B3lyp631pd_PCMdmso.log			-994.82868128	-994.497144	-994.476438	-994.475494	-994.547811	152.206
0308aba_Ph_NMeBn_CHC_COOMe_CN_product_B3lyp631pd_PCMdmso.log			-994.83455861	-994.502679	-994.482259	-994.481315	-994.552343	149.491
0308abb_Ph_NMeBn_CHC_COOMe_CN_product_B3lyp631pd_PCMdmso.log			-994.82940934	-994.497795	-994.477355	-994.476410	-994.547572	149.773
0401aaa_Ph_NMeBn_CHC_H_H_B3lyp631pd_PCMdmso.log			-674.69225799	-674.404056	-674.389112	-674.388168	-674.447023	123.871
0408aaa_Ph_NMeBn_CHC_H_H_product_B3lyp631pd_PCMdmso.log			-674.71915830	-674.428190	-674.414308	-674.413364	-674.469209	117.536
0501aaa_Ph_NMeBn_CHC_NO2_Me_B3lyp631pd_PCMdmso.log			-918.52156936	-918.202322	-918.183413	-918.182469	-918.251604	145.508
0502aaa_Ph_NMeBn_CHC_NO2_Me_ZW_INT_B3lyp631pd_PCMdmso.log			-918.48173014	-918.162393	-918.143343	-918.142398	-918.211434	145.297
0503daa_Ph_NMeBn_CHC_NO2_Me_ZW_INT_B3lyp631pd_PCMdmso_TS_CH.log			-918.46904569	-918.154454	-918.135865	-918.134921	-918.202737	142.730
0508aaa_Ph_NMeBn_CHC_NO2_Me_product_B3lyp631pd_PCMdmso.log			-918.54189897	-918.220248	-918.202383	-918.201439	-918.266195	136.291
0508aba_Ph_NMeBn_CHC_NO2_Me_product_B3lyp631pd_PCMdmso.log			-918.54189907	-918.220250	-918.202383	-918.201439	-918.266201	136.303
0508abb_Ph_NMeBn_CHC_NO2_Me_product_B3lyp631pd_PCMdmso.log			-918.53935849	-918.217830	-918.200036	-918.199092	-918.263501	135.560

Table S5 Computed energies (E), zero point energies, internal energies (U), enthalpies (H) and Gibbs free energies (G) given in Hartree as well as entropies (S) given in J mol^{-1} K^{-1} at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of the solvent applied.

			E	ZPE	U	H	G	S
0601aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMdmso.log			-859.17959000	-858.893297	-858.874910	-858.873966	-858.941730	142.622
0602dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso_TS_HC.log			-859.12909025	-858.847639	-858.829608	-858.828663	-858.895470	140.607
0603aaa_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log			-859.18965374	-858.902002	-858.884403	-858.883459	-858.947798	135.413
0603aab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log			-859.15279040	-858.866223	-858.847565	-858.846621	-858.916973	148.069
0611aaa_Ph_NMeBn_CHC_CN_CN_product_B3lyp631pd_PCMdmso.log			-859.18965381	-858.902003	-858.884404	-858.883459	-858.947800	135.416
0701aaa_Ph_NMeBn_CHC_CN_Me_B3lyp631pd_PCMdmso.log			-806.26130789	-805.945869	-805.927681	-805.926737	-805.993789	141.122
0702dab_Ph_NMeBn_CHC_CN_Me_ZWion_B3lyp631pd_PCMdmso_TS_CH.log			-806.18870683	-805.877520	-805.859743	-805.858799	-805.924053	137.340
0702fab_Ph_NMeBn_CHC_CN_Me_ZWion_B3lyp631pd_PCMdmso_SCAN_CH_vege.log			-806.26131492	-805.945794	-805.927588	-805.926644	-805.993681	141.090
0703aab_Ph_NMeBn_CHC_CN_Me_ZWion_B3lyp631pd_PCMdmso.log			-806.18973996	-805.876113	-805.857434	-805.856489	-805.925574	145.401
0711aaa_Ph_NMeBn_CHC_CN_Me_product_B3lyp631pd_PCMdmso.log			-806.27872374	-805.961301	-805.944116	-805.943172	-806.006125	132.497
0801aaa_Ph_NMeBn_CHC_Me_Me_B3lyp631pd_PCMdmso.log			-753.33292195	-752.988770	-752.970782	-752.969838	-753.035812	138.854
0803aab_Ph_NMeBn_CHC_Me_Me_ZWion_B3lyp631pd_PCMdmso.log			-753.22107840	-752.881453	-752.862880	-752.861936	-752.929596	142.404
0811aaa_Ph_NMeBn_CHC_Me_Me_product_B3lyp631pd_PCMdmso.log			-753.35499607	-753.008347	-752.991587	-752.990643	-753.052268	129.702
0901aaa_Ph_NMeBn_CHC_COOMe_COOMe_B3lyp631pd_PCMdmso.log			-1130.45362422	-1130.079616	-1130.055432	-1130.054488	-1130.136764	173.164
0901aab_Ph_NMeBn_CHC_COOMe_COOMe_B3lyp631pd_PCMdmso.log			-1130.45457390	-1130.080503	-1130.056394	-1130.055450	-1130.137371	172.416
0902dab_Ph_NMeBn_CHC_COOMe_COOMe_ZWion_B3lyp631pd_PCMdmso_TS_CH.log			-1130.39991971	-1130.030567	-1130.007073	-1130.006129	-1130.085277	166.580
0903aab_Ph_NMeBn_CHC_COOMe_COOMe_ZWion_B3lyp631pd_PCMdmso.log			-1130.42968339	-1130.055213	-1130.031371	-1130.030427	-1130.110089	167.663
0911aaa_Ph_NMeBn_CHC_COOMe_COOMe_product_B3lyp631pd_PCMdmso.log			-1130.46752131	-1130.091567	-1130.068350	-1130.067406	-1130.145115	163.551
1001aab_Ph_NMeBn_CHC_COOMe_H_B3lyp631pd_PCMdmso.log			-902.58196429	-902.250440	-902.231002	-902.230058	-902.300275	147.785
1002dab_Ph_NMeBn_CHC_COOMe_H_ZWion_B3lyp631pd_PCMdmso_TS_CH.log			-902.51105131	-902.181455	-902.162532	-902.161588	-902.230608	145.266
1003aab_Ph_NMeBn_CHC_COOMe_H_ZWion_B3lyp631pd_PCMdmso.log			-902.51223163	-902.182557	-902.162619	-902.161675	-902.234642	153.573
1011aaa_Ph_NMeBn_CHC_COOMe_H_product_B3lyp631pd_PCMdmso.log			-902.60313583	-902.269501	-902.250785	-902.249841	-902.317968	143.386
1101aab_Ph_NMeBn_CHC_NO2_NO2_B3lyp631pd_PCMdmso.log			-1083.67881727	-1083.385392	-1083.365325	-1083.364380	-1083.436926	152.685
1102dab_Ph_NMeBn_CHC_NO2_NO2_ZWion_B3lyp631pd_PCMdmso_TS_CH.log			-1083.66636212	-1083.373799	-1083.354335	-1083.353391	-1083.425065	150.850
1102fab_Ph_NMeBn_CHC_NO2_NO2_ZWion_B3lyp631pd_PCMdmso_SCAN_CH_vege.log			-1083.67891225	-1083.385597	-1083.365394	-1083.364450	-1083.438406	155.653
1103aab_Ph_NMeBn_CHC_NO2_NO2_ZWion_B3lyp631pd_PCMdmso.log			-1083.68859337	-1083.393996	-1083.374175	-1083.373231	-1083.444418	149.826
1111aaa_Ph_NMeBn_CHC_NO2_NO2_product_B3lyp631pd_PCMdmso.log			-1083.69962861	-1083.404209	-1083.385002	-1083.384058	-1083.452649	144.361

Table S6 Computed energies (E), zero point energies, internal energies (U), enthalpies (H) and Gibbs free energies (G) given in Hartree as well as entropies (S) given in J mol^{-1} K^{-1} at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of the solvent applied.

			E	ZPE	U	H	G	S
1201aab_Ph_NMeBn_CHC_NO2_H_B3lyp631pd_PCMdmso.log			-879.20166938	-878.910353	-878.892902	-878.891957	-878.957764	138.501
1202dab_Ph_NMeBn_CHC_NO2_H_ZWion_B3lyp631pd_PCMdmso_TS_CH.log			-879.14300488	-878.856355	-878.839411	-878.838466	-878.902612	135.006
1203aab_Ph_NMeBn_CHC_NO2_H_ZWion_B3lyp631pd_PCMdmso.log			-879.16199851	-878.870645	-878.853125	-878.852180	-878.918258	139.071
1211aaa_Ph_NMeBn_CHC_NO2_H_product_B3lyp631pd_PCMdmso.log			-879.22688764	-878.933080	-878.916455	-878.915511	-878.978678	132.947
1301aab_Ph_NMeBn_CHC_CF3_CF3_B3lyp631pd_PCMdmso.log			-1348.75910437	-1348.460912	-1348.438980	-1348.438036	-1348.514751	161.460
1302fab_Ph_NMeBn_CHC_CF3_CF3_ZW_INT_B3lyp631pd_PCMdmso_SCAN_CH_vege.log			-1348.70863617	-1348.411793	-1348.389471	-1348.388527	-1348.466438	163.978
1311aaa_Ph_NMeBn_CHC_CF3_CF3_product_B3lyp631pd_PCMdmso.log			-1348.78089942	-1348.480356	-1348.459724	-1348.458780	-1348.529377	148.584
1313aab_Ph_NMeBn_CHC_CF3_CF3_ZWion_B3lyp631pd_PCMdmso.log			-1348.70863619	-1348.411792	-1348.389471	-1348.388527	-1348.466428	163.957
251aa_model4_Naft_Pirrolidin_CN2_b3lyp631dp_PCMdmso.log			-859.18555497	-858.897632	-858.880157	-858.879213	-858.943912	136.170
253ab_model4_Naft_Pirrolidin_CN2_b3lyp631dp_PCMdmso_TS_2.log			-859.14921783	-858.864630	-858.847959	-858.847015	-858.909194	130.867
255ab_model4_Naft_Pirrolidin_CN2_INT_b3lyp631dp_PCMdmso.log			-859.15880391	-858.870661	-858.853247	-858.852303	-858.916576	135.274
256aa_model4_Naft_Pirrolidin_CN2_TERMEK1_b3lyp631dp_PCMdmso.log			-859.20343316	-858.912737	-858.896556	-858.895611	-858.955699	126.465
256ab_model4_Naft_Pirrolidin_CN2_TERMEK1_b3lyp631dp_PCMdmso.log			-859.19331776	-858.903001	-858.886568	-858.885624	-858.946804	128.764
1401_biphenylO_b3lyp631dp_PCMdmso.log			-1011.81971457	-1011.493576	-1011.472806	-1011.471862	-1011.546255	156.573
1404_biphenylO_ZWINT_b3lyp631dp_PCMdmso_TS_CH.log			-1011.77079408	-1011.448847	-1011.429093	-1011.428149	-1011.497896	146.794
1405_biphenylO_ZWINT_b3lyp631dp_PCMdmso.log			-1011.79847607	-1011.472592	-1011.451901	-1011.450957	-1011.524884	155.593
1409_biphenylO_PRODUCT_b3lyp631dp_PCMdmso.log			-1011.81134928	-1011.483606	-1011.464239	-1011.463294	-1011.530912	142.313
1411aab_biphenylO_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1011.81661419	-1011.488013	-1011.468942	-1011.467998	-1011.534755	140.502
1501aaa_model2_PhPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log			-936.60548679	-936.283335	-936.263628	-936.262684	-936.333304	148.632
1504aaa_model2_PhPh_pyrrolidine_CN2_TS_b3lyp631dp_PCMdmso_f.log			-936.56075759	-936.242971	-936.224099	-936.223155	-936.290691	142.141
1505aaa_model2_PhPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log			-936.58300659	-936.261493	-936.242421	-936.241476	-936.311295	146.946
1509aaa_model2_PhPh_pyrrolidine_CN2_PRODUCTb3lyp631dp_PCMdmso.log			-936.61301615	-936.288916	-936.270644	-936.269700	-936.334482	136.345
1509aab_model2_PhPh_pyrrolidine_CN2_PRODUCTb3lyp631dp_PCMdmso.log			-936.61301616	-936.288916	-936.270644	-936.269700	-936.334482	136.345
1509aac_model2_PhPh_pyrrolidine_CN2_PRODUCTb3lyp631dp_PCMdmso.log			-936.61369274	-936.289193	-936.270857	-936.269913	-936.335069	137.132
1601aab_model3_PhPhPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log			-1167.66277625	-1167.259990	-1167.235554	-1167.234610	-1167.316540	172.436
1604aad_model3_PhPhPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso_TS_CH_f.log			-1167.61799579	-1167.219137	-1167.195667	-1167.194723	-1167.272394	163.472
1605aad_model3_PhPhPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log			-1167.63698439	-1167.234154	-1167.209721	-1167.208777	-1167.290339	171.663
1609aaa_model3_PhPhPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1167.65003586	-1167.245157	-1167.222187	-1167.221243	-1167.296286	157.942
1511aab_model2_PhPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1167.65330832	-1167.247762	-1167.225026	-1167.224082	-1167.298540	156.711

Table S7. Computed energies (E), zero point energies, internal energies (U), enthalpies (H) and Gibbs free energies (G) given in Hartree as well as entropies (S) given in J mol^{-1} K^{-1} at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of the solvent applied.

			E	ZPE	U	H	G	S
1701aaa_model3_NaphtPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log			-1090.24293570	-1089.874138	-1089.851792	-1089.850848	-1089.926963	160.197
1701aab_model3_NaphtPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log			-1090.24335168	-1089.874540	-1089.852208	-1089.851264	-1089.927103	159.618
1704aab_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso_TS_CH_f2.log			-1090.18615205	-1089.821683	-1089.800182	-1089.799237	-1089.872158	153.475
1705aab_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log			-1090.21434501	-1089.845334	-1089.822960	-1089.822016	-1089.898925	161.869
1705aac_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log			-1090.21644900	-1089.847914	-1089.825356	-1089.824412	-1089.902103	163.514
1705aad_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log			-1090.21737876	-1089.848224	-1089.826150	-1089.825206	-1089.900137	157.707
1705aae_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log			-1090.21364709	-1089.845165	-1089.822561	-1089.821617	-1089.899741	164.426
1709aab_model3_NaphtPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1090.24534391	-1089.873982	-1089.852979	-1089.852035	-1089.922732	148.796
1709aac_model3_NaphtPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1090.24534391	-1089.873982	-1089.852979	-1089.852035	-1089.922732	148.795
1709aad_model3_NaphtPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1090.23880686	-1089.868070	-1089.847082	-1089.846138	-1089.917316	149.805
1801aaa_model4_PhOCH2Ph_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log			-1051.13350096	-1050.777781	-1050.755805	-1050.754861	-1050.832736	163.902
1801aaa_model4_PhOCH2Ph_pyrrolidine_CN2_b3lyp631dp_TS_PCMdmso.log			-1051.08491500	-1050.733132	-1050.712933	-1050.711989	-1050.782042	147.438
1805aaa_model4_PhOCH2Ph_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log			-1051.10618325	-1050.751106	-1050.728861	-1050.727917	-1050.806522	165.437
1809aaa_model4_PhOCH2Ph_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1051.12552492	-1050.768642	-1050.748107	-1050.747163	-1050.817385	147.794
1809aab_model4_PhOCH2Ph_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1051.11208096	-1050.754143	-1050.733897	-1050.732953	-1050.802077	145.484
1901aaa_model4_PhCH2OPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log			-1051.12769505	-1050.772474	-1050.750401	-1050.749457	-1050.827299	163.833
1901aab_model4_PhCH2OPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log			-1051.12728999	-1050.772140	-1050.750078	-1050.749134	-1050.826270	162.347
1904aaa_model4_PhCH2OPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso_TS_CH.log			-1051.08808453	-1050.736729	-1050.715836	-1050.714891	-1050.787284	152.364
1905aaa_model4_PhCH2OPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log			-1051.10931361	-1050.753855	-1050.731844	-1050.730900	-1050.807834	161.922
1909aaa_model4_PhCH2OPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1051.12544975	-1050.768202	-1050.747768	-1050.746823	-1050.816673	147.011
1909aab_model4_PhCH2OPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log			-1051.10712043	-1050.749488	-1050.728975	-1050.728031	-1050.798837	149.024
0601aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMdmso.log			-859.17959000	-858.893297	-858.874910	-858.873966	-858.941730	142.622
0602bbb_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log			-859.15297752	-858.866507	-858.847848	-858.846904	-858.917128	147.799
0602dcb_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso_TS_HC_f.log			-859.13536521	-858.853650	-858.835622	-858.834678	-858.901806	141.282
0603aaa_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log			-859.18965374	-858.902002	-858.884403	-858.883459	-858.947798	135.413
0603aab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log			-859.15279040	-858.866223	-858.847565	-858.846621	-858.916973	148.069
0609aaa_Ph_NMeBn_CHC_CN_CN_product_B3lyp631pd_PCMdmso.log			-859.18965381	-858.902003	-858.884404	-858.883459	-858.947800	135.416
0621aaa_Ph_NPiperidin_CHC_CN_CN_B3lyp631pd_PCMdmso.log		5	-705.54644629	-705.305045	-705.289960	-705.289016	-705.349046	126.343
0623aba_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso_TS_CH_vissza.log			-705.50572761	-705.268592	-705.254341	-705.253397	-705.310885	120.994
0624aaa_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso.log			-705.52552504	-705.284402	-705.269390	-705.268446	-705.328000	125.341
0629baa_Ph_NPiperidin_CHC_CN_CN_PRODUCT_B3lyp631pd_PCMdmso.log			-705.56515328	-705.322102	-705.308121	-705.307177	-705.362731	116.923
0631aaa_Ph_NPiperidin_CHC_CN_CN_B3lyp631pd_PCMdmso.log		6	-744.86959462	-744.598797	-744.583070	-744.582126	-744.642739	127.572
0632aba_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso_TS_CH.log			-744.82492313	-744.558431	-744.543230	-744.542286	-744.601669	124.981
0634aaa_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso.log			-744.84593632	-744.575510	-744.559455	-744.558510	-744.621191	131.923
0639baa_Ph_NPiperidin_CHC_CN_CN_PRODUCT_B3lyp631pd_PCMdmso.log			-744.87619096	-744.603677	-744.588883	-744.587939	-744.644947	119.983

Table S8 Computed energies (E), zero point energies, internal energies (U), enthalpies (H) and Gibbs free energies (G) given in Hartree as well as entropies (S) given in J mol^{-1} K^{-1} at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of the solvent applied.

			E	ZPE	U	H	G	S
0641aaa_Ph_NMorf_CHC_CN_CN_B3lyp631pd_PCMdmso.log		6	-780.75674763	-780.509823	-780.494371	-780.493427	-780.553543	126.524
0643abb_Ph_NMorf_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso_TS_CH.log			-780.70798076	-780.465577	-780.450617	-780.449673	-780.508806	124.457
0644aaa_Ph_NMorf_CHC_CN_CN_BZW_3lyp631pd_PCMdmso.log			-780.72488686	-780.478644	-780.462917	-780.461973	-780.523545	129.591
0649aba_Ph_NMorf_CHC_CN_CN_PR_3lyp631pd_PCMdmso.log			-780.76456759	-780.515967	-780.501461	-780.500517	-780.557087	119.061
0651aaa_Ph_NMeEt_CHC_CN_CN_B3lyp631pd_PCMdmso.log			-667.43947154	-667.206282	-667.190892	-667.189948	-667.249503	125.345
0653aaa_Ph_NMeEt_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso_TS_CH.log			-667.38953838	-667.161014	-667.146112	-667.145168	-667.203535	122.843
0654aaa_Ph_NMeEt_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso.log			-667.41368925	-667.180991	-667.165256	-667.164312	-667.225357	128.480
0659aba_Ph_NMeEt_CHC_CN_CN_PR_B3lyp631pd_PCMdmso.log			-667.45096643	-667.215713	-667.201456	-667.200512	-667.256393	117.612
0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMw.log			-859.17979920	-858.893504	-858.875118	-858.874174	-858.941929	142.603
0601aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMdmso.log			-859.17959000	-858.893297	-858.874910	-858.873966	-858.941730	142.622
0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMacn.log			-859.17943006	-858.893137	-858.874749	-858.873805	-858.941577	142.639
0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMdce.log			-859.17783608	-858.891567	-858.873169	-858.872225	-858.940128	142.916
0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMtol.log			-859.17228082	-858.886076	-858.867642	-858.866698	-858.934992	143.737
0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd.log			-859.16596983	-858.879710	-858.861292	-858.860347	-858.928536	143.516
0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMw_TS_HC.log		78.3553	-859.12943333	-858.847988	-858.829955	-858.829011	-858.895835	140.643
0602dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso_TS_HC.log		46.826	-859.12909025	-858.847639	-858.829608	-858.828663	-858.895470	140.607
0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMacn_TS_HC.log		35.688	-859.12882731	-858.847372	-858.829342	-858.828398	-858.895197	140.591
0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdce_TS_HC.log		10.125	-859.12618681	-858.844697	-858.826674	-858.825729	-858.892498	140.525
0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMtol_TS_HC.log		2.3741	-859.13358659	-858.847331	-858.829762	-858.828818	-858.893706	136.569
0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_TS_HC.log		1	-859.10456045	-858.822468	-858.804457	-858.803513	-858.870395	140.766
0662eab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMw_TS_HC.log		78.3553	-859.17256191	-858.886547	-858.868815	-858.867871	-858.933626	138.392
0602dcb_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso_TS_HC_f.log		46.826	-859.13536521	-858.853650	-858.835622	-858.834678	-858.901806	141.282
0662eab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMacn_TS_HC.log		35.688	-859.13510796	-858.853391	-858.835362	-858.834418	-858.901579	141.354
0662eab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdce_TS_HC_f.log		10.125	-859.13258184	-858.850736	-858.832794	-858.831850	-858.898451	140.173
0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMw.log			-859.15353706	-858.866983	-858.848317	-858.847373	-858.917835	148.300
0603aab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log			-859.15279040	-858.866223	-858.847565	-858.846621	-858.916973	148.069
0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMacn.log			-859.15221608	-858.865640	-858.846987	-858.846043	-858.916327	147.926
0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdce.log			-859.14635992	-858.859748	-858.841123	-858.840179	-858.910106	147.173
0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMtol.log			-859.13587176	-858.849403	-858.830945	-858.830001	-858.898029	143.177
0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd.log			-859.12655638	-858.840913	-858.822932	-858.821987	-858.888051	139.042

Table S9 Computed energies (E), zero point energies, internal energies (U), enthalpies (H) and Gibbs free energies (G) given in Hartree as well as entropies (S) given in J mol^{-1} K^{-1} at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of the solvent applied.

			E	ZPE	U	H	G	S
931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMw.log			-861.59775942	-861.264715	-861.245272	-861.244328	-861.314039	146.719
931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMdmso.log			-861.59742329	-861.264386	-861.244941	-861.243996	-861.313721	146.747
931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMacn.log			-861.59716693	-861.264134	-861.244687	-861.243742	-861.313482	146.779
931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMdce.log			-861.59465386	-861.261653	-861.242195	-861.241250	-861.311081	146.970
931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMtol.log			-861.58631368	-861.253449	-861.233927	-861.232983	-861.303189	147.761
931aa_model1B_chexene_Me_CN2_b3lyp631dp.log			-861.57743751	-861.244553	-861.225051	-861.224107	-861.294096	147.305
933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMw_TS_CH.log			-861.54522135	-861.217631	-861.198460	-861.197515	-861.266977	146.194
933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMdmso_TS_CH_f.log			-861.54500341	-861.217463	-861.198272	-861.197328	-861.266844	146.309
933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMacn_TS_CH.log			-861.54475732	-861.217198	-861.198013	-861.197069	-861.266553	146.241
933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMdce_TS_CH.log			-861.54227236	-861.214541	-861.195409	-861.194465	-861.263608	145.523
933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMtol_TS_CH.log			-861.53328584	-861.205202	-861.186152	-861.185208	-861.254072	144.936
933aa_model1B_chexene_Ph_CN2_b3lyp631dp_TS_CH_f.log			-861.52276109	-861.194336	-861.175348	-861.174404	-861.242729	143.803
951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMw.log			-862.80482442	-862.449131	-862.429244	-862.428300	-862.499700	150.274
951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMdmso.log			-862.80463166	-862.448931	-862.429047	-862.428103	-862.499472	150.210
951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMacn.log			-862.80448416	-862.448777	-862.428895	-862.427951	-862.499305	150.177
951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMdce.log			-862.80301456	-862.447265	-862.427396	-862.426452	-862.497660	149.871
951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMtol.log			-862.79786269	-862.442099	-862.422212	-862.421268	-862.492543	150.011
951aa_model1C_chexane_Ph_CN2_b3lyp631dp.log			-862.79192341	-862.436195	-862.416256	-862.415312	-862.486991	150.861
953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_PCMdmso_TS_CH_f2.log			-862.76180348	-862.409736	-862.390616	-862.389671	-862.458154	144.134
953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_PCMacn_TS_CH.log			-862.76153993	-862.409474	-862.390353	-862.389408	-862.457897	144.146
953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_PCMdce_TS_CH_f2.log			-862.75890022	-862.406833	-862.387703	-862.386759	-862.455258	144.169
953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_PCMtol_TS_CH.log			-862.74925720	-862.397143	-862.377991	-862.377047	-862.445713	144.521
953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_TS_CH.log			-862.73732726	-862.384858	-862.365728	-862.364783	-862.433440	144.499

The xyz coordinates of computed geometries (for labeling see Table S3-S7)

0001aaa_pentadiene_B3LYP631dp_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192870	0.569669	-0.110601
2	6	0	0.051433	1.082316	-0.073874
3	1	0	-2.003454	1.266583	-0.321141
4	1	0	0.143961	2.158989	-0.215997
5	6	0	1.321518	0.392797	0.186188
6	6	0	1.660667	-0.859172	-0.156921
7	1	0	2.074761	1.001748	0.688069
8	1	0	2.639260	-1.259670	0.090579
9	1	0	0.994721	-1.511168	-0.712790
10	6	0	-1.614056	-0.849464	0.136774
11	1	0	-1.806534	-1.380269	-0.805401
12	1	0	-0.853318	-1.415321	0.680961
13	1	0	-2.549553	-0.877770	0.706318

0001aba_pentadiene_B3LYP631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192876	0.569600	-0.110676
2	6	0	0.051393	1.082248	-0.073813
3	1	0	-2.003417	1.266467	-0.321535
4	1	0	0.144002	2.158897	-0.216050
5	6	0	1.321413	0.392720	0.186354
6	6	0	1.660811	-0.859008	-0.157267
7	1	0	2.074455	1.001558	0.688667
8	1	0	2.639380	-1.259496	0.090339
9	1	0	0.995186	-1.510765	-0.713792
10	6	0	-1.614087	-0.849466	0.136995
11	1	0	-1.806963	-1.380340	-0.805078
12	1	0	-0.853184	-1.415268	0.680995
13	1	0	-2.549388	-0.877615	0.706892

0001aca_pentadiene_B3LYP631dp_PCMmecn.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192877	0.569578	-0.110712
2	6	0	0.051372	1.082230	-0.073821
3	1	0	-2.003420	1.266420	-0.321646
4	1	0	0.143975	2.158874	-0.216093
5	6	0	1.321368	0.392709	0.186399
6	6	0	1.660830	-0.858954	-0.157341
7	1	0	2.074344	1.001495	0.688875
8	1	0	2.639372	-1.259462	0.090323
9	1	0	0.995300	-1.510616	-0.714081
10	6	0	-1.614056	-0.849476	0.137058
11	1	0	-1.806858	-1.380452	-0.804979
12	1	0	-0.853156	-1.415163	0.681178
13	1	0	-2.549379	-0.877620	0.706923

0001ada_pentadiene_B3LYP631dp_PCMdce.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192779	0.569335	-0.111604
2	6	0	0.051187	1.082158	-0.074181
3	1	0	-2.003404	1.265715	-0.323786
4	1	0	0.143866	2.158676	-0.217441
5	6	0	1.320609	0.392528	0.187750
6	6	0	1.660652	-0.858173	-0.158205
7	1	0	2.072275	1.000009	0.693774
8	1	0	2.638350	-1.259810	0.090849
9	1	0	0.996248	-1.507853	-0.718527
10	6	0	-1.613242	-0.849689	0.137633
11	1	0	-1.805235	-1.382186	-0.803743
12	1	0	-0.851998	-1.413580	0.683129
13	1	0	-2.548662	-0.877926	0.707393

0001aea_pentadiene_B3LYP631dp_PCMtol.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192633	0.567950	-0.115055
2	6	0	0.050520	1.081170	-0.075735
3	1	0	-2.003128	1.262570	-0.333539
4	1	0	0.143846	2.157039	-0.223677
5	6	0	1.318036	0.391342	0.194019
6	6	0	1.662547	-0.854406	-0.163037
7	1	0	2.062990	0.993587	0.716062
8	1	0	2.637068	-1.259767	0.092045
9	1	0	1.004398	-1.495886	-0.739877
10	6	0	-1.612251	-0.850083	0.140787
11	1	0	-1.812644	-1.384747	-0.797667
12	1	0	-0.846906	-1.412155	0.682160
13	1	0	-2.542944	-0.876485	0.718616

0001afa_pentadiene_B3LYP631dp_vacuo.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192507	0.566586	-0.118462
2	6	0	0.049775	1.080210	-0.077062
3	1	0	-2.002932	1.259423	-0.342829
4	1	0	0.143643	2.155478	-0.229085
5	6	0	1.315332	0.390196	0.199897
6	6	0	1.664319	-0.850610	-0.167597
7	1	0	2.053732	0.987154	0.737171
8	1	0	2.635739	-1.259465	0.093248
9	1	0	1.012585	-1.484136	-0.760180
10	6	0	-1.611028	-0.850526	0.143706
11	1	0	-1.819371	-1.387590	-0.791713
12	1	0	-0.841644	-1.410604	0.681188
13	1	0	-2.537101	-0.875389	0.729307

0001baa_pentadiene_TS_b3lyp631dp_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.211650	0.507912	-0.012029
2	6	0	-0.000328	1.184767	0.151236
3	1	0	2.045450	1.094931	-0.395980
4	1	0	-0.000547	2.269917	0.089046
5	6	0	-1.212192	0.507322	-0.012151
6	6	0	-1.310343	-0.906740	-0.022357
7	1	0	-2.046159	1.094023	-0.396152
8	1	0	-2.181755	-1.329318	-0.525247
9	1	0	-1.062055	-1.462840	0.879730
10	6	0	1.310907	-0.906424	-0.022680
11	1	0	1.063053	-1.462444	0.879629
12	1	0	0.000129	-1.197917	-0.498684
13	1	0	2.183721	-1.327377	-0.524453

0001bba_pentadiene_TS_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.211639	0.507789	-0.012070
2	6	0	-0.000264	1.184730	0.151343
3	1	0	2.045665	1.094731	-0.395563
4	1	0	-0.000400	2.269851	0.088925
5	6	0	-1.211995	0.507426	-0.012240
6	6	0	-1.310482	-0.906788	-0.022510
7	1	0	-2.046141	1.094034	-0.395947
8	1	0	-2.183031	-1.328561	-0.524041
9	1	0	-1.061777	-1.462645	0.879637
10	6	0	1.310878	-0.906455	-0.022742
11	1	0	1.062695	-1.462804	0.879261
12	1	0	0.000183	-1.197665	-0.499003
13	1	0	2.184151	-1.327154	-0.523958

0001bca_pentadiene_TS_b3lyp631dp_PCMacn.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.211350	0.508137	-0.011886
2	6	0	-0.000739	1.184712	0.151166
3	1	0	2.045415	1.095555	-0.394584
4	1	0	-0.001151	2.269866	0.089288
5	6	0	-1.212404	0.507069	-0.012453
6	6	0	-1.310152	-0.907090	-0.022261
7	1	0	-2.046680	1.093379	-0.396320
8	1	0	-2.182418	-1.329853	-0.523405
9	1	0	-1.060471	-1.462346	0.879992
10	6	0	1.311273	-0.906138	-0.022986
11	1	0	1.063766	-1.462917	0.878973
12	1	0	0.000626	-1.197817	-0.499191
13	1	0	2.184947	-1.326011	-0.524232

0001bda_pentadiene_TS_b3lyp631dp_PCMdce.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.211252	0.508083	-0.011942
2	6	0	-0.000710	1.184622	0.151126
3	1	0	2.045307	1.095371	-0.394845
4	1	0	-0.001119	2.269777	0.089421
5	6	0	-1.212270	0.507035	-0.012424
6	6	0	-1.309972	-0.907033	-0.022322
7	1	0	-2.046617	1.093303	-0.396190
8	1	0	-2.182170	-1.329868	-0.523500
9	1	0	-1.060649	-1.461931	0.880255
10	6	0	1.311049	-0.906109	-0.022949
11	1	0	1.063789	-1.462348	0.879417
12	1	0	0.000682	-1.197706	-0.499427
13	1	0	2.184680	-1.326186	-0.524070

0001bea_pentadiene_TS_b3lyp631dp_PCMtol.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.210872	0.507941	-0.012046
2	6	0	-0.000700	1.184321	0.150992
3	1	0	2.045006	1.094969	-0.395112
4	1	0	-0.001094	2.269478	0.089854
5	6	0	-1.211883	0.506901	-0.012447
6	6	0	-1.309328	-0.906897	-0.022425
7	1	0	-2.046392	1.092957	-0.396122
8	1	0	-2.181394	-1.330139	-0.523393
9	1	0	-1.061073	-1.460372	0.881336
10	6	0	1.310398	-0.905967	-0.022967
11	1	0	1.064091	-1.460652	0.880635
12	1	0	0.000733	-1.197506	-0.500140
13	1	0	2.183964	-1.326525	-0.523699

0001bfa_pentadiene_TS_b3lyp631dp_vacuo.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.210736	0.507575	-0.012390
2	6	0	-0.000293	1.184153	0.151131
3	1	0	2.044904	1.093939	-0.396401
4	1	0	-0.000432	2.269330	0.090692
5	6	0	-1.211122	0.507167	-0.012519
6	6	0	-1.308631	-0.906647	-0.022679
7	1	0	-2.045510	1.093178	-0.396551
8	1	0	-2.180719	-1.329966	-0.523543
9	1	0	-1.063290	-1.458387	0.883009
10	6	0	1.309066	-0.906263	-0.022861
11	1	0	1.064228	-1.458458	0.882705
12	1	0	0.000313	-1.197045	-0.500727
13	1	0	2.181964	-1.328499	-0.523278

0101aaa_Ph_NMeBn_CHC_H_CN_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.433556	-0.078016	0.218320
2	6	0	3.406894	0.856461	0.169537
3	6	0	2.065339	0.472161	-0.016300

4	6	0	1.749871	-0.915242	-0.123031
5	6	0	2.805235	-1.844285	-0.094537
6	6	0	4.125545	-1.432891	0.070927
7	1	0	5.461554	0.245223	0.344773
8	1	0	3.647134	1.913527	0.223230
9	1	0	2.592966	-2.902952	-0.177435
10	1	0	4.915082	-2.178185	0.095750
11	7	0	0.406198	-1.327609	-0.279800
12	6	0	-0.517495	-1.017664	0.824188
13	1	0	-0.146142	-0.131483	1.346116
14	1	0	-0.502393	-1.833425	1.566216
15	6	0	0.186362	-2.671158	-0.814192
16	1	0	-0.864407	-2.766625	-1.095012
17	1	0	0.794597	-2.824219	-1.707850
18	1	0	0.414317	-3.466541	-0.087127
19	6	0	-1.955179	-0.769564	0.394472
20	6	0	-2.979057	-0.906576	1.342459
21	6	0	-2.291885	-0.363556	-0.902382
22	6	0	-4.304637	-0.629551	1.008006
23	1	0	-2.734824	-1.231893	2.350995
24	6	0	-3.620066	-0.092166	-1.242015
25	1	0	-1.510629	-0.276176	-1.651008
26	6	0	-4.630415	-0.220126	-0.287981
27	1	0	-5.083776	-0.739819	1.756742
28	1	0	-3.862887	0.217456	-2.254498
29	1	0	-5.662617	-0.009709	-0.551746
30	6	0	1.021180	1.476488	-0.191896
31	6	0	1.061379	2.755252	0.250202
32	1	0	0.142250	1.152482	-0.742282
33	1	0	1.882732	3.137381	0.849159
34	6	0	0.018632	3.680318	-0.032779
35	7	0	-0.825416	4.455559	-0.249345

0101aaa_Ph_NMeBn_CHC_H_CN_ZW_INT_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.126570	-1.135888	0.598055
2	6	0	-3.344393	0.009047	0.676329
3	6	0	-1.972844	-0.004899	0.370348
4	6	0	-1.418626	-1.231574	-0.045145
5	6	0	-2.206978	-2.391287	-0.150978
6	6	0	-3.554267	-2.343865	0.173889
7	1	0	-5.178286	-1.094733	0.863890
8	1	0	-3.788204	0.955795	0.971519
9	1	0	-1.753485	-3.327674	-0.458633
10	1	0	-4.156192	-3.244581	0.109102
11	7	0	-0.022431	-1.298472	-0.376535
12	6	0	0.836178	-0.732922	0.474311
13	1	0	0.464488	-0.662499	1.490933
14	6	0	0.349125	-1.816971	-1.701324
15	1	0	1.366748	-2.203169	-1.673874
16	1	0	-0.332057	-2.625312	-1.960210
17	1	0	0.263287	-1.037221	-2.463595
18	6	0	2.229691	-0.393536	0.279828
19	6	0	3.021013	-0.313703	1.450838
20	6	0	2.835600	-0.091600	-0.962378
21	6	0	4.368845	0.014585	1.380043
22	1	0	2.565462	-0.522669	2.414197
23	6	0	4.182933	0.247037	-1.021659
24	1	0	2.252733	-0.083414	-1.873975
25	6	0	4.957020	0.292664	0.142205
26	1	0	4.960826	0.059202	2.288441
27	1	0	4.630619	0.484981	-1.981217
28	1	0	6.008780	0.554402	0.085427
29	6	0	-1.202876	1.305565	0.410679
30	6	0	-1.655366	2.254738	-0.634421
31	1	0	-1.310149	1.748430	1.408502
32	1	0	-1.797442	1.892877	-1.647749
33	6	0	-1.767000	3.613780	-0.408405
34	7	0	-1.874803	4.776436	-0.210800
35	1	0	-0.105382	1.072794	0.345294

0101daa_Ph_NMeBn_CHC_H_CN_ZW_INT_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.324258	-0.587308	-0.407184
2	6	0	3.378944	0.427828	-0.497971
3	6	0	2.008777	0.177096	-0.327343
4	6	0	1.611425	-1.144585	-0.026046
5	6	0	2.566792	-2.170197	0.084894
6	6	0	3.912955	-1.892697	-0.108541
7	1	0	5.375009	-0.368316	-0.569070
8	1	0	3.687966	1.448763	-0.703769
9	1	0	2.249761	-3.184165	0.302671
10	1	0	4.641676	-2.693839	-0.035111
11	7	0	0.230509	-1.418699	0.199366
12	6	0	-0.649006	-0.731378	-0.575773
13	1	0	-0.337532	-0.642608	-1.613975
14	6	0	-0.149918	-2.156567	1.410016
15	1	0	-1.177650	-2.502539	1.316643
16	1	0	0.499024	-3.025585	1.513718
17	1	0	-0.047260	-1.539850	2.308865
18	6	0	-2.072125	-0.539571	-0.320745
19	6	0	-2.934475	-0.508158	-1.438091
20	6	0	-2.620705	-0.305063	0.959126
21	6	0	-4.298872	-0.288363	-1.279117
22	1	0	-2.524534	-0.668499	-2.430920
23	6	0	-3.985610	-0.079257	1.109663
24	1	0	-1.978762	-0.268684	1.831245
25	6	0	-4.831023	-0.077023	-0.004013
26	1	0	-4.947304	-0.279485	-2.149539
27	1	0	-4.390500	0.104933	2.099809
28	1	0	-5.894998	0.097928	0.120682
29	6	0	1.031711	1.332445	-0.390311
30	6	0	1.229579	2.360471	0.615748
31	1	0	0.978790	1.742459	-1.406366
32	1	0	1.529598	2.076319	1.619213
33	6	0	0.888063	3.691139	0.399419
34	7	0	0.611990	4.822897	0.214536
35	1	0	-0.025402	0.820905	-0.323821

0108aaa_Ph_NMeBn_CHC_H_CN_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.663290	-0.211574	-0.284316
2	6	0	3.765362	0.850640	-0.281794
3	6	0	2.386771	0.646668	-0.118538
4	6	0	1.902744	-0.667641	0.027306
5	6	0	2.816592	-1.739232	0.019832
6	6	0	4.179939	-1.515720	-0.126761
7	1	0	5.726228	-0.028454	-0.407083
8	1	0	4.132292	1.868196	-0.393960
9	1	0	2.439278	-2.753135	0.110732
10	1	0	4.864773	-2.358594	-0.133279
11	7	0	0.512982	-0.943498	0.161139
12	6	0	-0.367073	0.137178	-0.313313
13	1	0	-0.134883	0.267621	-1.377257
14	6	0	0.124924	-1.605472	1.413955
15	1	0	-0.853344	-2.074926	1.304139
16	1	0	0.851268	-2.384403	1.644589
17	1	0	0.087108	-0.919031	2.275210
18	6	0	-1.838541	-0.238739	-0.226639
19	6	0	-2.649285	0.091544	0.867588
20	6	0	-2.403466	-0.963425	-1.285378
21	6	0	-3.992154	-0.290510	0.899754
22	1	0	-2.240838	0.646911	1.706286
23	6	0	-3.743516	-1.349477	-1.254969

24	1	0	-1.785529	-1.225281	-2.140150
25	6	0	-4.543058	-1.011953	-0.160494
26	1	0	-4.605596	-0.023570	1.755024
27	1	0	-4.163419	-1.907478	-2.086541
28	1	0	-5.587790	-1.306882	-0.135525
29	6	0	1.460780	1.845352	-0.104475
30	6	0	0.036385	1.483826	0.375164
31	1	0	1.876492	2.634617	0.529715
32	1	0	0.036198	1.342455	1.462544
33	6	0	-0.882237	2.584036	0.076117
34	7	0	-1.589502	3.469588	-0.180786
35	1	0	1.388653	2.266320	-1.115144

0108baa_Ph_NMeBn_CHC_H_CN_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.535231	-0.513936	-0.318231
2	6	0	3.684933	0.447586	-0.855017
3	6	0	2.298994	0.407050	-0.647600
4	6	0	1.747752	-0.648528	0.114005
5	6	0	2.617703	-1.613882	0.661112
6	6	0	3.989664	-1.547169	0.450539
7	1	0	5.605562	-0.457202	-0.489749
8	1	0	4.097957	1.266472	-1.439652
9	1	0	2.206617	-2.434495	1.238966
10	1	0	4.633211	-2.309673	0.879755
11	7	0	0.351211	-0.763323	0.322431
12	6	0	-0.473071	0.058317	-0.577339
13	1	0	-0.248533	-0.304302	-1.589406
14	6	0	-0.090095	-0.953048	1.711185
15	1	0	-1.168201	-1.107511	1.730680
16	1	0	0.373806	-1.848146	2.128356
17	1	0	0.156061	-0.103128	2.361341
18	6	0	-1.967034	-0.160085	-0.386230
19	6	0	-2.839044	0.819513	0.101607
20	6	0	-2.497048	-1.407668	-0.753087
21	6	0	-4.207649	0.558573	0.222162
22	1	0	-2.466312	1.794366	0.396761
23	6	0	-3.859357	-1.671753	-0.628918
24	1	0	-1.829556	-2.174815	-1.136026
25	6	0	-4.721644	-0.685598	-0.140376
26	1	0	-4.868178	1.332526	0.601386
27	1	0	-4.249535	-2.642554	-0.919820
28	1	0	-5.784620	-0.886496	-0.046874
29	6	0	1.436580	1.508001	-1.234312
30	6	0	0.018099	1.538648	-0.621085
31	1	0	1.928094	2.477872	-1.111774
32	1	0	-0.641388	2.123940	-1.270737
33	6	0	0.024314	2.199899	0.689473
34	7	0	0.041903	2.748759	1.713758
35	1	0	1.313246	1.359572	-2.313854

0201aaa_Ph_NMeBn_CHC_Me_COOMe_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.560300	-0.396355	-0.051380
2	6	0	3.487604	0.490881	-0.014528
3	6	0	2.156191	0.049489	-0.116818
4	6	0	1.905098	-1.349092	-0.243825
5	6	0	2.999110	-2.229433	-0.288125
6	6	0	4.309213	-1.760578	-0.196081
7	1	0	5.577851	-0.023999	0.011177
8	1	0	3.681745	1.556373	0.036338
9	1	0	2.829943	-3.295388	-0.379419
10	1	0	5.131886	-2.468973	-0.229891
11	7	0	0.570883	-1.818112	-0.353780

12	6	0	-0.294198	-1.592913	0.816946
13	1	0	0.013613	-0.657784	1.292148
14	1	0	-0.133458	-2.387351	1.565480
15	6	0	0.393441	-3.157777	-0.911723
16	1	0	-0.662467	-3.300081	-1.150282
17	1	0	0.969920	-3.259087	-1.833521
18	1	0	0.691928	-3.959427	-0.216885
19	6	0	-1.778051	-1.512609	0.496604
20	6	0	-2.709494	-1.890160	1.473230
21	6	0	-2.251548	-1.022482	-0.727153
22	6	0	-4.080406	-1.766918	1.241372
23	1	0	-2.357669	-2.283792	2.423917
24	6	0	-3.622795	-0.906657	-0.965639
25	1	0	-1.540036	-0.747020	-1.498637
26	6	0	-4.542527	-1.273983	0.018857
27	1	0	-4.786346	-2.063940	2.011651
28	1	0	-3.971946	-0.530423	-1.923116
29	1	0	-5.608727	-1.183712	-0.166908
30	6	0	1.046916	1.001541	-0.236047
31	6	0	0.880276	2.193141	0.385928
32	1	0	0.264386	0.689676	-0.920967
33	6	0	1.762316	2.761673	1.467982
34	1	0	2.374979	1.986661	1.931052
35	1	0	2.434274	3.536738	1.078986
36	1	0	1.147480	3.238417	2.235314
37	6	0	-0.293328	3.043191	0.041795
38	8	0	-0.558905	4.092050	0.610875
39	8	0	-1.050496	2.558215	-0.968019
40	6	0	-2.208839	3.338209	-1.310704
41	1	0	-2.696026	2.798421	-2.121640
42	1	0	-2.881903	3.426679	-0.454809
43	1	0	-1.916058	4.337664	-1.640513

0202aaa_Ph_NMeBn_CHC_Me_COOMe_ZW_INT_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.434594	3.394255	-0.711635
2	6	0	-2.279876	2.027492	-0.911433
3	6	0	-1.106084	1.348806	-0.541130
4	6	0	-0.093806	2.115346	0.064222
5	6	0	-0.243897	3.493294	0.291099
6	6	0	-1.411693	4.132562	-0.100158
7	1	0	-3.347086	3.889063	-1.029959
8	1	0	-3.082928	1.448176	-1.358852
9	1	0	0.563262	4.055112	0.750322
10	1	0	-1.522657	5.200336	0.058915
11	7	0	1.133519	1.474394	0.469180
12	6	0	1.756027	0.719291	-0.432010
13	1	0	1.481723	0.949753	-1.455777
14	6	0	1.498825	1.536560	1.889726
15	1	0	2.581409	1.483186	1.998573
16	1	0	1.141131	2.480781	2.295796
17	1	0	1.025160	0.719225	2.444661
18	6	0	2.841321	-0.222312	-0.266262
19	6	0	3.600129	-0.494060	-1.431082
20	6	0	3.176670	-0.907022	0.926267
21	6	0	4.668950	-1.380205	-1.397930
22	1	0	3.344069	0.007908	-2.359298
23	6	0	4.241930	-1.799922	0.946554
24	1	0	2.589425	-0.776090	1.824985
25	6	0	4.997489	-2.034778	-0.206883
26	1	0	5.243079	-1.565518	-2.299922
27	1	0	4.479650	-2.323416	1.866976
28	1	0	5.828698	-2.732098	-0.179538
29	6	0	-1.052080	-0.161170	-0.714509
30	6	0	-1.915731	-0.892686	0.252035
31	1	0	-1.368885	-0.415853	-1.730473
32	1	0	0.014189	-0.492697	-0.650745
33	6	0	-1.716500	-0.678035	1.726343
34	1	0	-0.758675	-1.093647	2.094542
35	1	0	-1.697940	0.388675	1.990653

36	1	0	-2.509911	-1.147506	2.310444
37	6	0	-2.787266	-1.870154	-0.272895
38	8	0	-2.984475	-2.151265	-1.475719
39	8	0	-3.496010	-2.572250	0.709668
40	6	0	-4.421449	-3.533855	0.216625
41	1	0	-4.886872	-3.984405	1.096164
42	1	0	-5.192583	-3.073237	-0.410471
43	1	0	-3.925199	-4.310825	-0.374512

0203daa_Ph_NMeBn_CHC_Me_COOMe_ZW_INT_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.477919	-3.362841	-0.685444
2	6	0	2.310073	-1.986693	-0.763506
3	6	0	1.086906	-1.363646	-0.459772
4	6	0	0.027039	-2.198621	-0.048466
5	6	0	0.193248	-3.591943	0.051659
6	6	0	1.411323	-4.171850	-0.268319
7	1	0	3.431258	-3.810247	-0.949429
8	1	0	3.139497	-1.349321	-1.058314
9	1	0	-0.641385	-4.215513	0.353993
10	1	0	1.529069	-5.248841	-0.204703
11	7	0	-1.242981	-1.621366	0.289501
12	6	0	-1.715840	-0.659996	-0.511868
13	1	0	-1.355961	-0.726540	-1.532914
14	6	0	-1.823580	-1.952710	1.597457
15	1	0	-2.900662	-1.795373	1.573169
16	1	0	-1.622592	-2.999783	1.814836
17	1	0	-1.374241	-1.344795	2.389564
18	6	0	-2.784076	0.287784	-0.274589
19	6	0	-3.445336	0.784466	-1.423818
20	6	0	-3.175052	0.786590	0.990613
21	6	0	-4.477456	1.707520	-1.311513
22	1	0	-3.144746	0.427073	-2.404307
23	6	0	-4.202618	1.717889	1.091902
24	1	0	-2.655656	0.480443	1.889314
25	6	0	-4.864434	2.175728	-0.051994
26	1	0	-4.978278	2.066085	-2.205074
27	1	0	-4.483383	2.096402	2.069610
28	1	0	-5.667401	2.900432	0.037458
29	6	0	1.015880	0.152921	-0.527721
30	6	0	1.980061	0.859541	0.343425
31	1	0	1.170864	0.478815	-1.562535
32	1	0	-0.047747	0.456625	-0.314953
33	6	0	2.122439	0.487409	1.797163
34	1	0	2.175500	1.372583	2.441308
35	1	0	1.270448	-0.115809	2.131988
36	1	0	3.024528	-0.105620	2.017789
37	6	0	2.694785	1.939068	-0.223212
38	8	0	2.632223	2.370601	-1.393928
39	8	0	3.557541	2.552599	0.687683
40	6	0	4.302291	3.651992	0.173535
41	1	0	4.919221	4.012073	0.999617
42	1	0	4.944647	3.351361	-0.660919
43	1	0	3.648343	4.458251	-0.175244

0208aaa_Ph_NMeBn_CHC_Me_COOMe_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.855612	0.172316	0.229242
2	6	0	3.783557	1.063837	0.295117
3	6	0	2.473496	0.660985	0.031034
4	6	0	2.205830	-0.693958	-0.280306
5	6	0	3.295155	-1.589882	-0.347949
6	6	0	4.596863	-1.158548	-0.098903
7	1	0	5.867328	0.510672	0.429483

8	1	0	3.962235	2.107639	0.543409
9	1	0	3.125573	-2.633486	-0.582969
10	1	0	5.410329	-1.876459	-0.158086
11	7	0	0.899473	-1.149250	-0.495292
12	6	0	-0.240345	-0.216003	-0.492254
13	1	0	-0.353281	0.234946	-1.488749
14	6	0	0.749012	-2.335190	-1.342984
15	1	0	-0.286872	-2.423855	-1.665338
16	1	0	1.384860	-2.271642	-2.235696
17	1	0	1.004260	-3.254426	-0.804482
18	6	0	-1.550915	-0.937433	-0.178119
19	6	0	-1.636938	-1.930185	0.809594
20	6	0	-2.713889	-0.589804	-0.878984
21	6	0	-2.855781	-2.544151	1.098758
22	1	0	-0.739635	-2.231632	1.339890
23	6	0	-3.936436	-1.199755	-0.587982
24	1	0	-2.660849	0.160739	-1.662570
25	6	0	-4.011788	-2.177995	0.404222
26	1	0	-2.901939	-3.312467	1.865154
27	1	0	-4.825169	-0.916135	-1.144100
28	1	0	-4.959566	-2.658246	0.628594
29	6	0	1.340421	1.655497	0.043138
30	6	0	0.020615	0.982048	0.493645
31	1	0	1.577387	2.491533	0.710409
32	1	0	1.198130	2.082108	-0.956334
33	6	0	0.115940	0.552333	1.965627
34	1	0	0.896119	-0.198865	2.099374
35	1	0	0.362099	1.417371	2.587001
36	1	0	-0.828320	0.142791	2.325296
37	6	0	-1.118669	1.999896	0.356008
38	8	0	-1.820665	2.391021	1.267746
39	8	0	-1.245284	2.451860	-0.908324
40	6	0	-2.276612	3.436330	-1.127978
41	1	0	-2.223950	3.683518	-2.187031
42	1	0	-3.256139	3.022945	-0.879345
43	1	0	-2.092100	4.322629	-0.517773

0208aba_Ph_NMeBn_CHC_Me_COOMe_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.855802	0.172430	0.228533
2	6	0	3.783707	1.063888	0.294685
3	6	0	2.473574	0.660909	0.031129
4	6	0	2.205900	-0.694066	-0.280036
5	6	0	3.295243	-1.589929	-0.347889
6	6	0	4.597012	-1.158494	-0.099313
7	1	0	5.867569	0.510849	0.428402
8	1	0	3.962381	2.107732	0.542795
9	1	0	3.125655	-2.633588	-0.582682
10	1	0	5.410485	-1.876382	-0.158676
11	7	0	0.899493	-1.149484	-0.494569
12	6	0	-0.240177	-0.216078	-0.491907
13	1	0	-0.352755	0.234817	-1.488471
14	6	0	0.748882	-2.335322	-1.342372
15	1	0	-0.287057	-2.423902	-1.664600
16	1	0	1.384573	-2.271693	-2.235204
17	1	0	1.004229	-3.254628	-0.804043
18	6	0	-1.550870	-0.937306	-0.178050
19	6	0	-1.637241	-1.929669	0.810054
20	6	0	-2.713526	-0.590008	-0.879548
21	6	0	-2.856193	-2.543459	1.099043
22	1	0	-0.740098	-2.230897	1.340755
23	6	0	-3.936208	-1.199825	-0.588733
24	1	0	-2.660151	0.160151	-1.663482
25	6	0	-4.011947	-2.177580	0.403893
26	1	0	-2.902690	-3.311430	1.865764
27	1	0	-4.824719	-0.916464	-1.145340
28	1	0	-4.959817	-2.657701	0.628150
29	6	0	1.340524	1.655490	0.043552
30	6	0	0.020674	0.982089	0.493933
31	1	0	1.577602	2.491304	0.711055

32	1	0	1.198297	2.082379	-0.955813
33	6	0	0.115769	0.552546	1.965987
34	1	0	0.895824	-0.198760	2.099874
35	1	0	0.362031	1.417628	2.587257
36	1	0	-0.828600	0.143235	2.325626
37	6	0	-1.118686	1.999828	0.355974
38	8	0	-1.820793	2.391100	1.267552
39	8	0	-1.245277	2.451480	-0.908466
40	6	0	-2.276835	3.435614	-1.128363
41	1	0	-2.224499	3.682284	-2.187552
42	1	0	-3.256224	3.022181	-0.879265
43	1	0	-2.092350	4.322283	-0.518679

0208abb_Ph_NMeBn_CHC_Me_COOMe_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.603961	-0.344152	-0.073008
2	6	0	-3.704016	0.482986	0.601490
3	6	0	-2.344474	0.180504	0.685874
4	6	0	-1.843769	-0.980801	0.053052
5	6	0	-2.760180	-1.817712	-0.621137
6	6	0	-4.116454	-1.500645	-0.680713
7	1	0	-5.658380	-0.090571	-0.119918
8	1	0	-4.062800	1.386381	1.090118
9	1	0	-2.413895	-2.716441	-1.115851
10	1	0	-4.790420	-2.167331	-1.211842
11	7	0	-0.479830	-1.288117	0.067889
12	6	0	0.474309	-0.508146	0.873765
13	1	0	0.493540	-0.908608	1.900782
14	6	0	-0.123186	-2.693497	-0.138680
15	1	0	0.923260	-2.846429	0.117566
16	1	0	-0.733460	-3.361035	0.484846
17	1	0	-0.249973	-2.991320	-1.185036
18	6	0	1.892166	-0.638396	0.315330
19	6	0	2.152139	-0.508856	-1.057325
20	6	0	2.967670	-0.876309	1.180595
21	6	0	3.455443	-0.597289	-1.546561
22	1	0	1.324208	-0.356673	-1.741875
23	6	0	4.274361	-0.961861	0.693634
24	1	0	2.781878	-1.001422	2.243971
25	6	0	4.522584	-0.819892	-0.672214
26	1	0	3.637454	-0.496487	-2.612623
27	1	0	5.094089	-1.147461	1.381442
28	1	0	5.536616	-0.890933	-1.054233
29	6	0	-1.421717	1.055195	1.492867
30	6	0	0.062684	0.999437	1.060986
31	1	0	-1.770631	2.093960	1.477694
32	1	0	-1.456982	0.744734	2.546154
33	6	0	0.918510	1.619857	2.180155
34	1	0	0.811138	1.037540	3.099770
35	1	0	1.974403	1.659472	1.910941
36	1	0	0.586067	2.641356	2.382134
37	6	0	0.280496	1.840420	-0.207361
38	8	0	1.071652	2.761170	-0.293764
39	8	0	-0.523723	1.481489	-1.223616
40	6	0	-0.400741	2.261602	-2.430432
41	1	0	-1.129632	1.843717	-3.123046
42	1	0	-0.620611	3.312152	-2.229884
43	1	0	0.608328	2.176264	-2.839195

0301aaa_Ph_NMeBn_CHC_COOMe_CN_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.440058	-0.789847	-0.156018
2	6	0	3.423454	0.151019	-0.095336
3	6	0	2.063536	-0.225001	-0.151841

4	6	0	1.729566	-1.615977	-0.225460
5	6	0	2.778816	-2.550041	-0.305879
6	6	0	4.108897	-2.143744	-0.273620
7	1	0	5.477761	-0.474678	-0.133726
8	1	0	3.678751	1.202958	-0.059281
9	1	0	2.555991	-3.607674	-0.364356
10	1	0	4.892878	-2.893445	-0.325027
11	7	0	0.383564	-2.025910	-0.241993
12	6	0	-0.460591	-1.667359	0.911448
13	1	0	-0.041004	-0.775895	1.384677
14	1	0	-0.405595	-2.465937	1.669142
15	6	0	0.105804	-3.380245	-0.722696
16	1	0	-0.966833	-3.471327	-0.902187
17	1	0	0.626753	-3.559471	-1.664890
18	1	0	0.395183	-4.157516	0.000916
19	6	0	-1.921458	-1.412117	0.573142
20	6	0	-2.873901	-1.486733	1.599347
21	6	0	-2.348188	-1.067871	-0.714698
22	6	0	-4.217595	-1.208611	1.348905
23	1	0	-2.559505	-1.764143	2.602715
24	6	0	-3.695565	-0.797863	-0.970334
25	1	0	-1.624519	-1.026248	-1.522512
26	6	0	-4.634052	-0.862862	0.060420
27	1	0	-4.940298	-1.269531	2.157416
28	1	0	-4.009758	-0.541157	-1.978001
29	1	0	-5.680933	-0.653551	-0.138208
30	6	0	1.007693	0.758533	-0.282346
31	6	0	0.959940	2.066762	0.110080
32	1	0	0.113896	0.402970	-0.785285
33	6	0	1.973591	2.708535	0.888045
34	7	0	2.785074	3.241463	1.531436
35	6	0	-0.202529	2.947749	-0.195715
36	8	0	-0.286506	4.102495	0.186475
37	8	0	-1.141538	2.330604	-0.930161
38	6	0	-2.313726	3.111337	-1.239711
39	1	0	-2.785943	3.469381	-0.323014
40	1	0	-2.046917	3.963315	-1.868460
41	1	0	-2.978517	2.434296	-1.772935

0301daa_Ph_NMeBn_CHC_COOMe_CN_ZW_INT_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.139870	-1.537260	-0.605629
2	6	0	3.230654	-0.503998	-0.809034
3	6	0	1.856363	-0.691780	-0.598598
4	6	0	1.418204	-1.951886	-0.132494
5	6	0	2.336096	-2.989690	0.082738
6	6	0	3.689245	-2.784013	-0.157525
7	1	0	5.194964	-1.375230	-0.801497
8	1	0	3.576246	0.468527	-1.146526
9	1	0	1.981205	-3.955749	0.425701
10	1	0	4.392104	-3.596009	-0.000874
11	7	0	0.039061	-2.125499	0.180959
12	6	0	-0.818357	-1.422306	-0.638500
13	1	0	-0.636956	-1.623134	-1.695464
14	6	0	-0.289876	-2.499747	1.562006
15	1	0	-1.344460	-2.762541	1.627693
16	1	0	0.303494	-3.372075	1.836397
17	1	0	-0.064899	-1.692257	2.269338
18	6	0	-2.227531	-1.125710	-0.308720
19	6	0	-3.206965	-1.397946	-1.280947
20	6	0	-2.615746	-0.507421	0.895111
21	6	0	-4.545841	-1.097572	-1.040401
22	1	0	-2.914712	-1.855998	-2.221223
23	6	0	-3.954388	-0.200927	1.127107
24	1	0	-1.871614	-0.246832	1.639598
25	6	0	-4.922831	-0.500482	0.164851
26	1	0	-5.292743	-1.325196	-1.794288
27	1	0	-4.241127	0.279001	2.057399
28	1	0	-5.965223	-0.260944	0.350572
29	6	0	0.906416	0.452524	-0.814221

30	6	0	0.986690	1.602593	0.041155
31	1	0	0.767798	0.731695	-1.861925
32	1	0	-0.209613	-0.139915	-0.679976
33	6	0	0.523308	2.882895	-0.468590
34	8	0	0.109543	3.079020	-1.608284
35	8	0	0.601956	3.875262	0.459873
36	6	0	0.173486	5.172853	0.019632
37	1	0	0.297571	5.830958	0.879251
38	1	0	0.786090	5.523334	-0.814881
39	1	0	-0.873704	5.152457	-0.292319
40	6	0	1.374284	1.467675	1.391259
41	7	0	1.690239	1.322476	2.509771

0302aaa_Ph_NMeBn_CHC_COOMe_CN_ZW_INT_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.454070	3.381314	-0.189701
2	6	0	-2.310264	2.145336	-0.815231
3	6	0	-1.198169	1.317674	-0.583646
4	6	0	-0.237486	1.807088	0.318682
5	6	0	-0.365428	3.044070	0.957302
6	6	0	-1.477744	3.839066	0.698559
7	1	0	-3.328273	3.990930	-0.397076
8	1	0	-3.079848	1.779673	-1.486142
9	1	0	0.411366	3.383289	1.635286
10	1	0	-1.575945	4.805364	1.181816
11	7	0	0.942898	1.011858	0.641343
12	6	0	1.877403	0.883768	-0.259847
13	1	0	1.731091	1.500243	-1.143254
14	6	0	0.999272	0.434755	2.001603
15	1	0	2.038118	0.355041	2.319391
16	1	0	0.458220	1.107965	2.664101
17	1	0	0.521776	-0.548491	2.004996
18	6	0	3.069222	0.063979	-0.231065
19	6	0	4.146354	0.512659	-1.027756
20	6	0	3.187620	-1.153616	0.475852
21	6	0	5.337253	-0.201487	-1.063225
22	1	0	4.044331	1.429875	-1.599360
23	6	0	4.374621	-1.874134	0.408406
24	1	0	2.342717	-1.566161	1.013812
25	6	0	5.452614	-1.394022	-0.342532
26	1	0	6.167602	0.159570	-1.660273
27	1	0	4.458096	-2.817965	0.936469
28	1	0	6.377527	-1.960721	-0.380957
29	6	0	-1.130481	-0.046086	-1.264432
30	6	0	-1.722868	-1.179726	-0.440754
31	1	0	-1.691162	0.034632	-2.200828
32	1	0	-0.101722	-0.290983	-1.542245
33	6	0	-3.128566	-1.374455	-0.468799
34	8	0	-3.947497	-0.712566	-1.125468
35	8	0	-3.554747	-2.428579	0.324561
36	6	0	-4.960466	-2.675563	0.311212
37	1	0	-5.124017	-3.508420	0.997424
38	1	0	-5.525965	-1.801675	0.649072
39	1	0	-5.312647	-2.948479	-0.688761
40	6	0	-0.882666	-1.981820	0.326976
41	7	0	-0.121501	-2.621474	0.963536

0308aaa_Ph_NMeBn_CHC_COOMe_CN_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.860776	0.067868	-0.554430
2	6	0	3.812903	0.978035	-0.461202
3	6	0	2.485862	0.560755	-0.290695
4	6	0	2.199778	-0.821310	-0.212411
5	6	0	3.268485	-1.737364	-0.312555

6	6	0	4.576846	-1.299336	-0.475499
7	1	0	5.880422	0.415898	-0.684906
8	1	0	4.018803	2.044730	-0.509195
9	1	0	3.064382	-2.802185	-0.286752
10	1	0	5.376324	-2.030370	-0.553634
11	7	0	0.875264	-1.280382	-0.068754
12	6	0	-0.176703	-0.310604	-0.366589
13	1	0	-0.048683	-0.011497	-1.412417
14	6	0	0.584587	-2.374955	0.864311
15	1	0	-0.163516	-3.051999	0.446167
16	1	0	1.494506	-2.943805	1.042971
17	1	0	0.223895	-2.013812	1.834874
18	6	0	-1.579231	-0.892710	-0.260942
19	6	0	-2.363587	-0.832479	0.898827
20	6	0	-2.103931	-1.531705	-1.394283
21	6	0	-3.641282	-1.396843	0.921312
22	1	0	-1.990020	-0.347886	1.793882
23	6	0	-3.376216	-2.101630	-1.371206
24	1	0	-1.507548	-1.581978	-2.301295
25	6	0	-4.150512	-2.034006	-0.210529
26	1	0	-4.235972	-1.337494	1.827772
27	1	0	-3.764213	-2.590816	-2.259511
28	1	0	-5.143936	-2.471724	-0.190209
29	6	0	1.401174	1.611945	-0.186320
30	6	0	0.080234	1.049452	0.415678
31	1	0	1.750858	2.459418	0.411289
32	1	0	1.149532	2.006313	-1.175704
33	6	0	-1.074023	2.041228	0.215224
34	8	0	-1.726151	2.539051	1.108983
35	8	0	-1.265308	2.274516	-1.088117
36	6	0	-2.344353	3.178930	-1.420632
37	1	0	-2.345211	3.239986	-2.507025
38	1	0	-3.292420	2.780865	-1.055116
39	1	0	-2.161795	4.159803	-0.978776
40	6	0	0.261001	0.830802	1.858364
41	7	0	0.452656	0.659180	2.990485

0308aba_Ph_NMeBn_CHC_COOMe_CN_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.863325	0.224158	0.063199
2	6	0	3.783551	1.104335	0.118684
3	6	0	2.473296	0.673503	-0.100072
4	6	0	2.213715	-0.694562	-0.352951
5	6	0	3.313040	-1.578263	-0.408359
6	6	0	4.613255	-1.121888	-0.205027
7	1	0	5.874706	0.581704	0.226916
8	1	0	3.953458	2.158489	0.323886
9	1	0	3.154261	-2.631725	-0.600075
10	1	0	5.433728	-1.832156	-0.253780
11	7	0	0.906377	-1.180152	-0.517572
12	6	0	-0.228504	-0.253240	-0.586573
13	1	0	-0.312927	0.192449	-1.587938
14	6	0	0.757994	-2.425728	-1.277812
15	1	0	-0.289363	-2.575600	-1.530682
16	1	0	1.340422	-2.399629	-2.207881
17	1	0	1.080835	-3.290704	-0.690211
18	6	0	-1.555738	-0.936617	-0.269294
19	6	0	-1.691205	-1.817372	0.814061
20	6	0	-2.678524	-0.657944	-1.059485
21	6	0	-2.927399	-2.393124	1.106069
22	1	0	-0.823711	-2.061072	1.417624
23	6	0	-3.917380	-1.231789	-0.764911
24	1	0	-2.582381	0.007621	-1.912610
25	6	0	-4.045161	-2.099255	0.320471
26	1	0	-3.016953	-3.075315	1.946193
27	1	0	-4.776892	-1.006395	-1.388918
28	1	0	-5.006071	-2.550425	0.548775
29	6	0	1.339226	1.666045	-0.082952
30	6	0	0.022470	0.978444	0.365406
31	1	0	1.567562	2.505046	0.580833

32	1	0	1.159142	2.084421	-1.078465
33	6	0	-1.156435	1.967567	0.283632
34	8	0	-1.839390	2.304878	1.226100
35	8	0	-1.305290	2.418817	-0.966183
36	6	0	-2.375754	3.371253	-1.174205
37	1	0	-2.333209	3.625671	-2.231200
38	1	0	-3.335142	2.915506	-0.924224
39	1	0	-2.214677	4.255804	-0.556172
40	6	0	0.156037	0.552969	1.769416
41	7	0	0.311595	0.228120	2.872260

0308abb_Ph_NMeBn_CHC_COOMe_CN_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.662655	-0.252874	-0.090424
2	6	0	3.713865	0.663716	-0.542979
3	6	0	2.361549	0.331901	-0.641078
4	6	0	1.919922	-0.951386	-0.248864
5	6	0	2.886548	-1.874962	0.203855
6	6	0	4.233795	-1.527470	0.279230
7	1	0	5.710321	0.023368	-0.029156
8	1	0	4.024887	1.661821	-0.842254
9	1	0	2.587494	-2.868358	0.512549
10	1	0	4.948206	-2.264471	0.635022
11	7	0	0.562309	-1.299730	-0.269397
12	6	0	-0.438371	-0.419878	-0.878428
13	1	0	-0.464036	-0.571304	-1.969422
14	6	0	0.253474	-2.732093	-0.341625
15	1	0	-0.800883	-2.867791	-0.572326
16	1	0	0.846207	-3.231716	-1.118954
17	1	0	0.446394	-3.228095	0.614652
18	6	0	-1.841677	-0.693667	-0.340933
19	6	0	-2.073466	-0.889504	1.028454
20	6	0	-2.928540	-0.724760	-1.222975
21	6	0	-3.367670	-1.099544	1.503731
22	1	0	-1.233782	-0.896777	1.715773
23	6	0	-4.225245	-0.931669	-0.747138
24	1	0	-2.760712	-0.589724	-2.287775
25	6	0	-4.448151	-1.117755	0.617765
26	1	0	-3.531777	-1.253360	2.566080
27	1	0	-5.056997	-0.954789	-1.444691
28	1	0	-5.454979	-1.283967	0.988765
29	6	0	1.391481	1.331668	-1.213774
30	6	0	-0.063455	1.110197	-0.713007
31	1	0	1.705991	2.354763	-0.987165
32	1	0	1.371002	1.249858	-2.307028
33	6	0	-0.271056	1.662114	0.714835
34	8	0	-1.100068	2.503586	0.994917
35	8	0	0.583966	1.126740	1.586387
36	6	0	0.492705	1.617366	2.945057
37	1	0	1.263143	1.081649	3.495836
38	1	0	0.676719	2.692672	2.968882
39	1	0	-0.495422	1.404449	3.356311
40	6	0	-0.962912	1.880541	-1.591699
41	7	0	-1.623118	2.472233	-2.339967

0401aaa_Ph_NMeBn_CHC_H_H_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.411605	0.082810	0.206908
2	6	0	3.456201	1.087838	0.076050
3	6	0	2.092634	0.799810	-0.096900
4	6	0	1.679966	-0.562721	-0.122705
5	6	0	2.656873	-1.566474	-0.006340
6	6	0	4.005902	-1.250588	0.152886
7	1	0	5.460127	0.338282	0.324937

8	1	0	3.771534	2.126764	0.061947
9	1	0	2.362241	-2.608914	-0.023229
10	1	0	4.735003	-2.050977	0.240710
11	7	0	0.304383	-0.882965	-0.292281
12	6	0	-0.587283	-0.469198	0.802641
13	1	0	-0.189805	0.453844	1.233710
14	1	0	-0.572875	-1.218411	1.613038
15	6	0	0.002855	-2.234704	-0.758324
16	1	0	-1.046823	-2.276972	-1.056839
17	1	0	0.616493	-2.476361	-1.628849
18	1	0	0.163132	-3.006996	0.012049
19	6	0	-2.027903	-0.227032	0.381331
20	6	0	-3.052126	-0.374368	1.326692
21	6	0	-2.365240	0.192941	-0.911657
22	6	0	-4.378621	-0.094689	0.994982
23	1	0	-2.807873	-0.710671	2.331617
24	6	0	-3.692888	0.466223	-1.249008
25	1	0	-1.582124	0.288328	-1.657168
26	6	0	-4.704201	0.327640	-0.296327
27	1	0	-5.157946	-0.214100	1.742229
28	1	0	-3.936172	0.786357	-2.258242
29	1	0	-5.736508	0.539803	-0.558600
30	6	0	1.122632	1.887028	-0.320071
31	6	0	1.218081	3.141949	0.139911
32	1	0	0.258127	1.617932	-0.923103
33	1	0	2.030317	3.466049	0.784894
34	1	0	0.471549	3.888011	-0.113542

0408aaa_Ph_NMeBn_CHC_H_H_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.531474	-0.197858	-0.264565
2	6	0	3.695046	0.910658	-0.357086
3	6	0	2.305832	0.805873	-0.188890
4	6	0	1.745881	-0.465247	0.058335
5	6	0	2.597283	-1.583967	0.147366
6	6	0	3.972788	-1.454373	-0.003904
7	1	0	5.604051	-0.087002	-0.392678
8	1	0	4.122223	1.892906	-0.548157
9	1	0	2.159475	-2.563109	0.318164
10	1	0	4.607211	-2.333396	0.065910
11	7	0	0.340819	-0.658574	0.197846
12	6	0	-0.465032	0.459038	-0.355194
13	1	0	-0.229540	0.471378	-1.429247
14	6	0	-0.076270	-1.142711	1.520967
15	1	0	-1.098031	-1.523136	1.473905
16	1	0	0.575892	-1.961206	1.827794
17	1	0	-0.030775	-0.366652	2.302449
18	6	0	-1.956608	0.171812	-0.251976
19	6	0	-2.812388	0.888718	0.592382
20	6	0	-2.502646	-0.848747	-1.046015
21	6	0	-4.178733	0.595608	0.641890
22	1	0	-2.419255	1.683022	1.218559
23	6	0	-3.863603	-1.146450	-0.997542
24	1	0	-1.847795	-1.413222	-1.704616
25	6	0	-4.708646	-0.422028	-0.151336
26	1	0	-4.826407	1.165010	1.302328
27	1	0	-4.266528	-1.938171	-1.622663
28	1	0	-5.770182	-0.648396	-0.114204
29	6	0	1.440924	2.050520	-0.269084
30	6	0	0.006546	1.806713	0.213380
31	1	0	1.908440	2.859640	0.303756
32	1	0	1.410654	2.399080	-1.310899
33	1	0	-0.031837	1.785701	1.309096
34	1	0	-0.644425	2.622214	-0.116789

0501aaa_Ph_NMeBn_CHC_NO2_Me_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.304801	-1.007261	0.068605
2	6	0	3.408529	0.053872	0.009849
3	6	0	2.021680	-0.158174	-0.114875
4	6	0	1.526217	-1.496252	-0.157368
5	6	0	2.449492	-2.554706	-0.109196
6	6	0	3.817465	-2.314020	0.001012
7	1	0	5.370406	-0.817151	0.142890
8	1	0	3.788248	1.069164	-0.006725
9	1	0	2.097853	-3.578557	-0.136808
10	1	0	4.502990	-3.155249	0.043120
11	7	0	0.136361	-1.727907	-0.274171
12	6	0	-0.706587	-1.262085	0.841612
13	1	0	-0.235187	-0.379150	1.281134
14	1	0	-0.729107	-2.025228	1.637388
15	6	0	-0.270426	-3.050139	-0.750204
16	1	0	-1.328991	-3.014828	-1.014334
17	1	0	0.297261	-3.317648	-1.643477
18	1	0	-0.137826	-3.839389	0.006537
19	6	0	-2.134769	-0.915750	0.452483
20	6	0	-3.142986	-1.002951	1.422186
21	6	0	-2.473593	-0.463133	-0.828618
22	6	0	-4.455073	-0.631528	1.125735
23	1	0	-2.897635	-1.364057	2.418112
24	6	0	-3.787837	-0.098979	-1.130707
25	1	0	-1.706737	-0.411969	-1.594624
26	6	0	-4.782514	-0.177483	-0.154212
27	1	0	-5.222106	-0.704725	1.891320
28	1	0	-4.033248	0.245296	-2.131323
29	1	0	-5.804163	0.105836	-0.389412
30	6	0	1.104482	0.950284	-0.354596
31	6	0	1.157600	2.205132	0.143501
32	1	0	0.279396	0.736508	-1.026630
33	7	0	0.161293	3.147340	-0.378000
34	8	0	0.170717	4.293402	0.090982
35	8	0	-0.636576	2.788387	-1.253782
36	6	0	2.055492	2.772714	1.197277
37	1	0	2.589912	1.967772	1.702045
38	1	0	2.789850	3.469386	0.778581
39	1	0	1.470540	3.326397	1.934898

0502aaa_Ph_NMeBn_CHC_NO2_Me_ZW_INT_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.970295	-2.605262	-0.585929
2	6	0	2.700718	-1.246090	-0.691577
3	6	0	1.454299	-0.706521	-0.318711
4	6	0	0.496569	-1.613700	0.160139
5	6	0	0.759718	-2.984950	0.290710
6	6	0	1.999151	-3.482836	-0.086962
7	1	0	3.939785	-2.988008	-0.890442
8	1	0	3.443084	-0.552288	-1.076187
9	1	0	-0.013050	-3.650716	0.661568
10	1	0	2.202978	-4.545196	-0.003492
11	7	0	-0.829966	-1.150416	0.545519
12	6	0	-1.597512	-0.624182	-0.372930
13	1	0	-1.194438	-0.708657	-1.378115
14	6	0	-1.198696	-1.299429	1.965864
15	1	0	-2.268714	-1.478308	2.056674
16	1	0	-0.648209	-2.146916	2.368067
17	1	0	-0.912362	-0.401655	2.519374
18	6	0	-2.889128	0.015821	-0.267203
19	6	0	-3.616272	0.094473	-1.478201
20	6	0	-3.441524	0.588376	0.901777
21	6	0	-4.875794	0.678427	-1.510599
22	1	0	-3.187030	-0.318209	-2.385795
23	6	0	-4.692373	1.190811	0.853198
24	1	0	-2.888932	0.605845	1.830666
25	6	0	-5.415882	1.225971	-0.343757

26	1	0	-5.429871	0.718612	-2.441995
27	1	0	-5.103900	1.640425	1.750313
28	1	0	-6.394976	1.693523	-0.368371
29	6	0	1.261389	0.804662	-0.419486
30	6	0	2.297842	1.597942	0.328381
31	1	0	1.316945	1.084735	-1.476339
32	1	0	0.267302	1.087294	-0.057368
33	7	0	3.372150	2.040163	-0.327344
34	8	0	3.573963	1.738845	-1.578174
35	8	0	4.239078	2.780884	0.280671
36	6	0	2.156809	1.943520	1.779684
37	1	0	1.276658	1.449759	2.203937
38	1	0	3.032431	1.636629	2.366484
39	1	0	2.045036	3.024878	1.947438

0503daa_Ph_NMeBn_CHC_NO2_Me_ZW_INT_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.161334	-1.231135	-0.469802
2	6	0	3.276836	-0.166910	-0.606789
3	6	0	1.893197	-0.337482	-0.445287
4	6	0	1.415632	-1.624835	-0.103825
5	6	0	2.310945	-2.696709	0.044128
6	6	0	3.673306	-2.501132	-0.141181
7	1	0	5.224223	-1.076158	-0.625010
8	1	0	3.648707	0.823253	-0.853510
9	1	0	1.933835	-3.683980	0.287042
10	1	0	4.354355	-3.339735	-0.036972
11	7	0	0.025804	-1.804288	0.138825
12	6	0	-0.803775	-1.007324	-0.612115
13	1	0	-0.568502	-1.039285	-1.676254
14	6	0	-0.382744	-2.443302	1.395087
15	1	0	-1.443029	-2.685248	1.350653
16	1	0	0.177035	-3.370164	1.518893
17	1	0	-0.187308	-1.803049	2.262588
18	6	0	-2.217275	-0.738148	-0.303445
19	6	0	-3.146074	-0.801311	-1.359727
20	6	0	-2.666342	-0.341760	0.971912
21	6	0	-4.491184	-0.514903	-1.139857
22	1	0	-2.808281	-1.086961	-2.351525
23	6	0	-4.010784	-0.049646	1.184618
24	1	0	-1.962497	-0.237858	1.790191
25	6	0	-4.927836	-0.141147	0.133308
26	1	0	-5.196841	-0.580091	-1.961968
27	1	0	-4.342598	0.258544	2.171028
28	1	0	-5.975190	0.087121	0.304494
29	6	0	0.978054	0.847268	-0.594702
30	6	0	1.154837	1.962278	0.285075
31	1	0	0.839753	1.165929	-1.630518
32	1	0	-0.141009	0.320151	-0.459950
33	7	0	0.736333	3.202945	-0.167167
34	8	0	0.238080	3.338028	-1.324934
35	8	0	0.866337	4.199234	0.601752
36	6	0	1.621886	1.881652	1.704936
37	1	0	1.813852	0.841739	1.977823
38	1	0	2.546129	2.448919	1.868042
39	1	0	0.876987	2.295462	2.394792

0508aaa_Ph_NMeBn_CHC_NO2_Me_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.729979	-0.132789	0.285187
2	6	0	3.766554	0.870994	0.189174
3	6	0	2.424757	0.577732	-0.062729
4	6	0	2.010546	-0.769164	-0.189699
5	6	0	2.991975	-1.779161	-0.093644

6	6	0	4.328371	-1.460874	0.137200
7	1	0	5.769497	0.117518	0.470850
8	1	0	4.056763	1.913429	0.295651
9	1	0	2.710387	-2.820556	-0.186440
10	1	0	5.056512	-2.264049	0.206912
11	7	0	0.662322	-1.106592	-0.375484
12	6	0	-0.356757	-0.064658	-0.564038
13	1	0	-0.380584	0.263542	-1.613035
14	6	0	0.391064	-2.385273	-1.042015
15	1	0	-0.648000	-2.415943	-1.363237
16	1	0	1.031133	-2.517749	-1.923587
17	1	0	0.551592	-3.231865	-0.366759
18	6	0	-1.756011	-0.564362	-0.208623
19	6	0	-1.989252	-1.392040	0.900033
20	6	0	-2.846693	-0.171974	-0.995984
21	6	0	-3.282857	-1.804629	1.218786
22	1	0	-1.150576	-1.725765	1.502286
23	6	0	-4.143129	-0.580564	-0.674989
24	1	0	-2.681308	0.457194	-1.865941
25	6	0	-4.365178	-1.397088	0.434428
26	1	0	-3.445121	-2.447911	2.078573
27	1	0	-4.975482	-0.266570	-1.297685
28	1	0	-5.371590	-1.720806	0.682300
29	6	0	1.417548	1.687038	-0.229759
30	6	0	0.038360	1.215256	0.257932
31	1	0	1.726932	2.575112	0.330716
32	1	0	1.331899	1.980584	-1.281287
33	7	0	-0.969937	2.301348	-0.157241
34	8	0	-1.010640	2.604804	-1.350807
35	8	0	-1.678840	2.814058	0.702715
36	6	0	-0.008201	1.047503	1.771674
37	1	0	0.296088	1.974203	2.262876
38	1	0	-1.004000	0.780546	2.121971
39	1	0	0.688538	0.259207	2.062058

0508aba_Ph_NMeBn_CHC_NO2_Me_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.729998	-0.132698	0.285117
2	6	0	3.766565	0.871029	0.188874
3	6	0	2.424787	0.577709	-0.063056
4	6	0	2.010507	-0.769177	-0.189859
5	6	0	2.991992	-1.779165	-0.093503
6	6	0	4.328341	-1.460820	0.137380
7	1	0	5.769518	0.117610	0.470737
8	1	0	4.056698	1.913503	0.295199
9	1	0	2.710489	-2.820591	-0.186076
10	1	0	5.056471	-2.263990	0.207318
11	7	0	0.662274	-1.106569	-0.375736
12	6	0	-0.356780	-0.064621	-0.564234
13	1	0	-0.380674	0.263656	-1.613193
14	6	0	0.390927	-2.385522	-1.041614
15	1	0	-0.647943	-2.416098	-1.363511
16	1	0	1.031422	-2.518756	-1.922761
17	1	0	0.550813	-3.231825	-0.365822
18	6	0	-1.756088	-0.564145	-0.208749
19	6	0	-1.989253	-1.391410	0.900256
20	6	0	-2.846775	-0.172239	-0.996315
21	6	0	-3.282783	-1.804116	1.219120
22	1	0	-1.150472	-1.724673	1.502622
23	6	0	-4.143145	-0.580959	-0.675211
24	1	0	-2.681484	0.456649	-1.866487
25	6	0	-4.365113	-1.397095	0.434511
26	1	0	-3.444947	-2.447110	2.079140
27	1	0	-4.975556	-0.267357	-1.298029
28	1	0	-5.371502	-1.720874	0.682399
29	6	0	1.417490	1.687044	-0.230074
30	6	0	0.038598	1.215109	0.257837
31	1	0	1.726973	2.575132	0.330316
32	1	0	1.331737	1.980575	-1.281607
33	7	0	-0.970086	2.301357	-0.157064

34	8	0	-1.011023	2.604884	-1.350530
35	8	0	-1.678760	2.813957	0.703091
36	6	0	-0.007725	1.047231	1.771576
37	1	0	0.297008	1.973766	2.262757
38	1	0	-1.003559	0.780600	2.121964
39	1	0	0.688690	0.258594	2.061812

0508abb_Ph_NMeBn_CHC_NO2_Me_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.648455	-0.235011	-0.155531
2	6	0	-3.739013	0.760387	0.201502
3	6	0	-2.378980	0.490888	0.363492
4	6	0	-1.889066	-0.815861	0.141635
5	6	0	-2.816550	-1.820112	-0.212466
6	6	0	-4.171674	-1.529882	-0.358311
7	1	0	-5.702495	-0.003573	-0.271111
8	1	0	-4.088256	1.776429	0.370869
9	1	0	-2.481474	-2.833819	-0.389543
10	1	0	-4.854030	-2.328580	-0.635465
11	7	0	-0.522713	-1.108338	0.230146
12	6	0	0.427183	-0.135889	0.787069
13	1	0	0.410267	-0.186405	1.887917
14	6	0	-0.167127	-2.516546	0.427853
15	1	0	0.889875	-2.597019	0.670138
16	1	0	-0.745828	-2.968189	1.244885
17	1	0	-0.340824	-3.099916	-0.481717
18	6	0	1.859759	-0.435366	0.344209
19	6	0	2.172791	-0.697149	-0.998139
20	6	0	2.892770	-0.439761	1.290093
21	6	0	3.490463	-0.943388	-1.382913
22	1	0	1.379280	-0.721393	-1.737782
23	6	0	4.213245	-0.682946	0.905257
24	1	0	2.662805	-0.258237	2.336566
25	6	0	4.515768	-0.933831	-0.433607
26	1	0	3.716178	-1.145860	-2.425714
27	1	0	5.000422	-0.683631	1.653196
28	1	0	5.540663	-1.128259	-0.735037
29	6	0	-1.454341	1.583735	0.828889
30	6	0	0.031223	1.357174	0.510352
31	1	0	-1.765591	2.554412	0.428244
32	1	0	-1.515308	1.678116	1.920351
33	7	0	0.241875	1.667898	-0.980000
34	8	0	-0.489552	1.099172	-1.789426
35	8	0	1.129083	2.457023	-1.300513
36	6	0	0.900306	2.313673	1.326422
37	1	0	1.956485	2.221596	1.078385
38	1	0	0.590736	3.346282	1.151637
39	1	0	0.766894	2.090878	2.387838

0601aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.182038	-0.898410	-0.052076
2	6	0	3.262955	0.135963	-0.089091
3	6	0	1.872103	-0.113686	-0.153823
4	6	0	1.403630	-1.469454	-0.119498
5	6	0	2.360931	-2.502478	-0.111814
6	6	0	3.721345	-2.220979	-0.078836
7	1	0	5.244928	-0.684431	-0.026529
8	1	0	3.619709	1.157779	-0.128605
9	1	0	2.039158	-3.535666	-0.094079
10	1	0	4.430443	-3.043029	-0.055362
11	7	0	0.031384	-1.750779	-0.117664
12	6	0	-0.811649	-1.173363	0.943334
13	1	0	-0.278802	-0.331794	1.393392

14	1	0	-0.934820	-1.914913	1.748421
15	6	0	-0.383034	-3.108855	-0.473817
16	1	0	-1.458184	-3.103465	-0.661178
17	1	0	0.121021	-3.430563	-1.386732
18	1	0	-0.180770	-3.837004	0.325607
19	6	0	-2.187458	-0.711034	0.486928
20	6	0	-3.164788	-0.453469	1.459316
21	6	0	-2.507411	-0.501017	-0.859101
22	6	0	-4.425761	0.017294	1.096040
23	1	0	-2.934300	-0.621649	2.508650
24	6	0	-3.773535	-0.034518	-1.225959
25	1	0	-1.767901	-0.716973	-1.624164
26	6	0	-4.735122	0.229268	-0.250908
27	1	0	-5.169037	0.213841	1.863201
28	1	0	-4.005020	0.118980	-2.275957
29	1	0	-5.718552	0.591261	-0.535371
30	6	0	0.923119	0.942836	-0.403958
31	6	0	1.010573	2.293087	-0.167421
32	1	0	-0.004271	0.624235	-0.871367
33	6	0	-0.043815	3.156257	-0.607073
34	7	0	-0.897406	3.865385	-0.960226
35	6	0	2.072753	2.943208	0.535576
36	7	0	2.913901	3.503891	1.114055

0602bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.811940	2.745128	0.469403
2	6	0	-2.879485	1.377615	0.200820
3	6	0	-1.750925	0.642448	-0.179116
4	6	0	-0.543209	1.354982	-0.269225
5	6	0	-0.451087	2.721542	0.002271
6	6	0	-1.596155	3.422681	0.375421
7	1	0	-3.711068	3.280474	0.758643
8	1	0	-3.819479	0.845483	0.300792
9	1	0	0.505400	3.225640	-0.091105
10	1	0	-1.534072	4.484835	0.587293
11	7	0	0.680337	0.666789	-0.673415
12	6	0	1.623712	0.510635	0.218734
13	1	0	1.356960	0.900642	1.196719
14	6	0	0.789046	0.286898	-2.097191
15	1	0	1.721295	0.678863	-2.506796
16	1	0	0.753150	-0.798254	-2.207208
17	1	0	-0.049329	0.732145	-2.626933
18	6	0	2.942870	-0.066710	0.126783
19	6	0	3.746736	0.132398	1.276307
20	6	0	3.477482	-0.802440	-0.958228
21	6	0	5.044692	-0.356182	1.330413
22	1	0	3.341882	0.680694	2.120986
23	6	0	4.773036	-1.297486	-0.888311
24	1	0	2.891457	-1.014001	-1.839714
25	6	0	5.560022	-1.071230	0.246212
26	1	0	5.650255	-0.187403	2.214021
27	1	0	5.171894	-1.866203	-1.721146
28	1	0	6.572245	-1.460610	0.286518
29	6	0	-1.831178	-0.858777	-0.470543
30	6	0	-3.023039	-1.599866	0.106064
31	1	0	-1.837260	-0.996069	-1.559617
32	6	0	-4.121776	-1.920438	-0.694480
33	7	0	-5.037820	-2.192528	-1.384753
34	6	0	-3.032743	-1.973288	1.453155
35	7	0	-3.015210	-2.283933	2.589597
36	1	0	-0.900832	-1.325989	-0.123388

0602bbb_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.869544	2.634952	-0.803722
2	6	0	-2.917902	1.331746	-0.308672
3	6	0	-1.773054	0.674056	0.156530
4	6	0	-0.569213	1.396082	0.090349
5	6	0	-0.495620	2.696737	-0.413798
6	6	0	-1.656510	3.321969	-0.863675
7	1	0	-3.781173	3.111363	-1.151027
8	1	0	-3.856166	0.787384	-0.294119
9	1	0	0.460386	3.209757	-0.439939
10	1	0	-1.609110	4.332438	-1.255574
11	7	0	0.673202	0.795725	0.567831
12	6	0	1.570073	0.443997	-0.315814
13	1	0	1.223413	0.532426	-1.341598
14	6	0	0.837503	0.699905	2.031325
15	1	0	1.357285	-0.222033	2.289580
16	1	0	1.390732	1.568116	2.397142
17	1	0	-0.151915	0.702335	2.481906
18	6	0	2.913191	-0.060090	-0.151990
19	6	0	3.458935	-0.671904	-1.305956
20	6	0	3.710320	0.036747	1.012923
21	6	0	4.738428	-1.210400	-1.284731
22	1	0	2.863142	-0.729457	-2.211420
23	6	0	4.996776	-0.486840	1.016355
24	1	0	3.354601	0.547118	1.896295
25	6	0	5.508230	-1.119501	-0.122005
26	1	0	5.139069	-1.689180	-2.171451
27	1	0	5.606900	-0.398167	1.908593
28	1	0	6.512613	-1.530292	-0.104794
29	6	0	-1.842653	-0.756451	0.696788
30	6	0	-2.960259	-1.626537	0.149714
31	1	0	-0.872936	-1.240007	0.526999
32	6	0	-2.861512	-2.166803	-1.135743
33	7	0	-2.752412	-2.615218	-2.219834
34	6	0	-4.093818	-1.902913	0.917004
35	7	0	-5.040905	-2.135275	1.579514
36	1	0	-1.956264	-0.706945	1.787541

0602dcb_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso_TS_HC_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.196431	-0.894909	-0.564980
2	6	0	-3.260293	0.108822	-0.786808
3	6	0	-1.887527	-0.122779	-0.609293
4	6	0	-1.473254	-1.396636	-0.152396
5	6	0	-2.422467	-2.403950	0.080914
6	6	0	-3.772652	-2.155474	-0.129132
7	1	0	-5.249899	-0.700379	-0.737724
8	1	0	-3.581594	1.091957	-1.117039
9	1	0	-2.095294	-3.382909	0.413253
10	1	0	-4.495700	-2.946578	0.041757
11	7	0	-0.099167	-1.614479	0.133039
12	6	0	0.772901	-0.896965	-0.663613
13	1	0	0.593455	-1.063546	-1.727543
14	6	0	0.252056	-2.108670	1.470353
15	1	0	1.305388	-2.382278	1.490256
16	1	0	0.049772	-1.363726	2.248427
17	1	0	-0.339328	-2.999099	1.683377
18	6	0	2.190913	-0.654406	-0.321484
19	6	0	3.166242	-0.921514	-1.298516
20	6	0	2.589992	-0.090767	0.905012
21	6	0	4.512183	-0.668813	-1.041606
22	1	0	2.865804	-1.337892	-2.255434
23	6	0	3.935439	0.168093	1.153914
24	1	0	1.848460	0.163880	1.654482
25	6	0	4.899717	-0.125497	0.185386
26	1	0	5.256258	-0.891584	-1.799694
27	1	0	4.231178	0.606341	2.101765
28	1	0	5.947587	0.077087	0.383778
29	6	0	-0.913842	0.995757	-0.848945
30	6	0	-1.008236	2.179719	-0.037292

31	1	0	-0.736076	1.208997	-1.905789
32	6	0	-0.511888	3.416135	-0.510405
33	7	0	-0.106287	4.436588	-0.914987
34	6	0	-1.461321	2.121880	1.301100
35	7	0	-1.832821	2.069833	2.409669
36	1	0	0.198728	0.375978	-0.661183

0602fab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso_scan_HC_vege.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.525447	3.179005	0.378050
2	6	0	-2.082003	1.910146	0.362873
3	6	0	-1.435650	0.836637	-0.291297
4	6	0	-0.151912	1.053680	-0.888700
5	6	0	0.374632	2.357641	-0.890434
6	6	0	-0.301956	3.400895	-0.267543
7	1	0	-2.046379	3.996449	0.864698
8	1	0	-3.057009	1.754184	0.808448
9	1	0	1.336837	2.547839	-1.350072
10	1	0	0.137963	4.393667	-0.267673
11	7	0	0.526794	-0.022404	-1.480568
12	6	0	0.942103	-1.161813	-0.620609
13	1	0	0.143153	-1.359366	0.095525
14	6	0	1.489062	0.286481	-2.537951
15	1	0	2.442866	0.685344	-2.166874
16	1	0	1.702844	-0.634117	-3.088266
17	1	0	1.050771	1.006802	-3.231372
18	6	0	2.250213	-0.945824	0.122642
19	6	0	2.293025	-0.147316	1.275811
20	6	0	3.437812	-1.534117	-0.331217
21	6	0	3.494655	0.062028	1.952915
22	1	0	1.379336	0.306108	1.650178
23	6	0	4.642636	-1.328141	0.345156
24	1	0	3.418007	-2.164061	-1.217024
25	6	0	4.673761	-0.527275	1.487934
26	1	0	3.510308	0.678820	2.846753
27	1	0	5.553317	-1.794558	-0.019117
28	1	0	5.608539	-0.367075	2.016960
29	6	0	-2.084373	-0.430525	-0.525516
30	6	0	-3.104938	-1.046552	0.155206
31	1	0	-1.709881	-0.970434	-1.392265
32	6	0	-3.650747	-2.271825	-0.345609
33	7	0	-4.096955	-3.269672	-0.747265
34	6	0	-3.672536	-0.582358	1.383213
35	7	0	-4.147741	-0.236757	2.388744
36	1	0	1.024607	-2.042382	-1.265822

0603aaa_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.660614	-0.134293	-0.112511
2	6	0	3.731878	0.885182	0.088129
3	6	0	2.374691	0.612359	0.273246
4	6	0	1.908372	-0.721905	0.226521
5	6	0	2.856059	-1.747145	0.022308
6	6	0	4.207603	-1.453519	-0.141288
7	1	0	5.712328	0.097191	-0.244861
8	1	0	4.060320	1.921038	0.116225
9	1	0	2.537974	-2.780751	-0.020303
10	1	0	4.907583	-2.269238	-0.297309
11	7	0	0.542597	-1.035081	0.343846
12	6	0	-0.433648	0.001267	0.684276
13	1	0	-0.426212	0.221661	1.763123
14	6	0	0.216744	-2.389019	0.808860
15	1	0	-0.835178	-2.438221	1.080782
16	1	0	0.388306	-3.128921	0.021371

17	1	0	0.816486	-2.664847	1.685316
18	6	0	-1.856321	-0.383354	0.295040
19	6	0	-2.904678	-0.124106	1.186573
20	6	0	-2.146735	-0.966078	-0.947254
21	6	0	-4.223091	-0.425683	0.839635
22	1	0	-2.689550	0.311855	2.158280
23	6	0	-3.463524	-1.269059	-1.292438
24	1	0	-1.339733	-1.195581	-1.634667
25	6	0	-4.505371	-0.996687	-0.402000
26	1	0	-5.024991	-0.220264	1.542056
27	1	0	-3.675168	-1.722153	-2.256196
28	1	0	-5.529481	-1.235871	-0.672020
29	6	0	1.413987	1.742508	0.538450
30	6	0	-0.001436	1.368988	0.014541
31	1	0	1.314181	1.945179	1.610651
32	6	0	0.025959	1.273229	-1.459677
33	7	0	0.076718	1.223300	-2.617424
34	6	0	-0.957652	2.427425	0.387769
35	7	0	-1.675018	3.281867	0.705138
36	1	0	1.752329	2.667651	0.065552

0603aab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.811940	-2.745128	0.469403
2	6	0	2.879485	-1.377615	0.200820
3	6	0	1.750925	-0.642448	-0.179116
4	6	0	0.543209	-1.354982	-0.269225
5	6	0	0.451087	-2.721542	0.002271
6	6	0	1.596155	-3.422681	0.375421
7	1	0	3.711068	-3.280474	0.758643
8	1	0	3.819479	-0.845483	0.300792
9	1	0	-0.505400	-3.225640	-0.091105
10	1	0	1.534072	-4.484835	0.587293
11	7	0	-0.680337	-0.666789	-0.673415
12	6	0	-1.623712	-0.510635	0.218734
13	1	0	-1.356960	-0.900642	1.196719
14	6	0	-0.789046	-0.286898	-2.097191
15	1	0	-1.721295	-0.678863	-2.506796
16	1	0	-0.753150	0.798254	-2.207208
17	1	0	0.049329	-0.732145	-2.626933
18	6	0	-2.942870	0.066710	0.126783
19	6	0	-3.746736	-0.132398	1.276307
20	6	0	-3.477482	0.802440	-0.958228
21	6	0	-5.044692	0.356182	1.330413
22	1	0	-3.341882	-0.680694	2.120986
23	6	0	-4.773036	1.297486	-0.888311
24	1	0	-2.891457	1.014001	-1.839714
25	6	0	-5.560022	1.071230	0.246212
26	1	0	-5.650255	0.187403	2.214021
27	1	0	-5.171894	1.866203	-1.721146
28	1	0	-6.572245	1.460610	0.286518
29	6	0	1.831178	0.858777	-0.470543
30	6	0	3.023039	1.599866	0.106064
31	1	0	1.837260	0.996069	-1.559617
32	6	0	4.121776	1.920438	-0.694480
33	7	0	5.037820	2.192528	-1.384753
34	6	0	3.032743	1.973288	1.453155
35	7	0	3.015210	2.283933	2.589597
36	1	0	0.900832	1.325989	-0.123388

0609aaa_Ph_NMeBn_CHC_CN_CN_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.660626	-0.134130	0.112851
2	6	0	3.731861	0.885307	-0.087726

3	6	0	2.374705	0.612435	-0.273081
4	6	0	1.908448	-0.721867	-0.226696
5	6	0	2.856193	-1.747061	-0.022545
6	6	0	4.207692	-1.453398	0.141311
7	1	0	5.712303	0.097404	0.245398
8	1	0	4.060211	1.921200	-0.115598
9	1	0	2.538207	-2.780703	0.019853
10	1	0	4.907676	-2.269111	0.297317
11	7	0	0.542662	-1.035043	-0.344122
12	6	0	-0.433577	0.001148	-0.684435
13	1	0	-0.426308	0.221549	-1.763305
14	6	0	0.216765	-2.389092	-0.809033
15	1	0	-0.835363	-2.438385	-1.080078
16	1	0	0.815944	-2.664624	-1.685939
17	1	0	0.389047	-3.128872	-0.021623
18	6	0	-1.856225	-0.383446	-0.295098
19	6	0	-2.904615	-0.124229	-1.186529
20	6	0	-2.146562	-0.966170	0.947287
21	6	0	-4.223054	-0.425717	-0.839452
22	1	0	-2.689564	0.311643	-2.158293
23	6	0	-3.463287	-1.269043	1.292585
24	1	0	-1.339431	-1.195713	1.634525
25	6	0	-4.505236	-0.996614	0.402201
26	1	0	-5.024973	-0.220289	-1.541849
27	1	0	-3.675002	-1.722097	2.256347
28	1	0	-5.529308	-1.235735	0.672426
29	6	0	1.413929	1.742534	-0.538230
30	6	0	-0.001417	1.368988	-0.014672
31	1	0	1.752192	2.667670	-0.065208
32	6	0	0.025672	1.273186	1.459642
33	7	0	0.076048	1.223244	2.617401
34	1	0	1.314387	1.945447	-1.610428
35	6	0	-0.957675	2.427472	-0.387886
36	7	0	-1.675208	3.281628	-0.705637

0621aaa_Ph_NPiperidin_CHC_CN_CN_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.504888	3.296133	-0.140619
2	6	0	-1.156647	2.073291	-0.143078
3	6	0	-0.433116	0.859758	-0.170793
4	6	0	0.998668	0.897297	-0.130755
5	6	0	1.636816	2.150748	-0.166936
6	6	0	0.895482	3.327429	-0.171281
7	1	0	-1.075837	4.218290	-0.142630
8	1	0	-2.238967	2.049674	-0.184425
9	1	0	2.718327	2.205314	-0.162263
10	1	0	1.415140	4.280887	-0.183498
11	7	0	1.717453	-0.299029	-0.084401
12	6	0	1.567684	-1.212558	1.075850
13	1	0	0.534393	-1.533435	1.209114
14	1	0	1.880766	-0.693681	1.995371
15	6	0	3.155443	-0.300344	-0.387439
16	1	0	3.337314	0.125155	-1.377633
17	1	0	3.721559	0.291934	0.350076
18	6	0	-1.067497	-0.414045	-0.404250
19	6	0	-2.353581	-0.825418	-0.158091
20	1	0	-0.420632	-1.157041	-0.865433
21	6	0	-2.773924	-2.127428	-0.580254
22	7	0	-3.120944	-3.186084	-0.919313
23	6	0	-3.341221	-0.061268	0.539418
24	7	0	-4.163758	0.530435	1.113560
25	6	0	2.525400	-2.373609	0.750462
26	6	0	3.535511	-1.785379	-0.274838
27	1	0	3.424064	-2.277382	-1.244633
28	1	0	4.574845	-1.905438	0.039735
29	1	0	1.979619	-3.214602	0.315071
30	1	0	3.015382	-2.734576	1.657852

0623aba_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso_TS_CH_vissza.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.423199	3.310299	-0.233125
2	6	0	0.476836	2.280670	-0.485367
3	6	0	0.054633	0.944789	-0.573202
4	6	0	-1.319017	0.672678	-0.361402
5	6	0	-2.223491	1.706853	-0.075481
6	6	0	-1.776246	3.019945	-0.018410
7	1	0	-0.073907	4.337279	-0.203979
8	1	0	1.530219	2.499121	-0.630749
9	1	0	-3.269199	1.469785	0.089218
10	1	0	-2.480677	3.819028	0.188867
11	7	0	-1.734915	-0.669620	-0.335207
12	6	0	-1.015107	-1.606967	-1.009325
13	1	0	-0.846050	-1.449807	-2.073216
14	6	0	-2.521863	-1.261395	0.778439
15	1	0	-2.434300	-0.638341	1.670042
16	1	0	-3.575198	-1.308074	0.482797
17	6	0	1.064576	-0.146170	-0.803753
18	6	0	2.241702	-0.178863	0.042110
19	1	0	1.311369	-0.287397	-1.859729
20	6	0	3.443115	-0.744810	-0.435336
21	7	0	4.437805	-1.207847	-0.845880
22	6	0	2.190336	0.201925	1.400737
23	7	0	2.150178	0.518462	2.527733
24	6	0	-1.327643	-2.976058	-0.459919
25	6	0	-1.903981	-2.662069	0.936135
26	1	0	-1.097409	-2.630242	1.673949
27	1	0	-2.639044	-3.398570	1.264202
28	1	0	-0.451048	-3.627542	-0.438895
29	1	0	-2.069643	-3.452677	-1.113855
30	1	0	0.359512	-1.184492	-0.687776

0624aaa_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.503365	2.458924	0.113926
2	6	0	-2.328720	1.244352	-0.549822
3	6	0	-1.085668	0.598369	-0.595999
4	6	0	-0.021535	1.240390	0.059843
5	6	0	-0.173527	2.458653	0.723740
6	6	0	-1.425810	3.070006	0.755711
7	1	0	-3.482155	2.928096	0.128385
8	1	0	-3.174661	0.775523	-1.044013
9	1	0	0.682381	2.918152	1.207276
10	1	0	-1.552644	4.013545	1.275622
11	7	0	1.309111	0.661973	0.033065
12	6	0	1.849385	-0.032021	0.979803
13	1	0	1.292602	-0.271354	1.877041
14	6	0	2.269275	0.954841	-1.078729
15	1	0	1.772660	0.782836	-2.034139
16	1	0	2.533103	2.013947	-1.007257
17	6	0	-0.949134	-0.758725	-1.273112
18	6	0	-1.040420	-1.940686	-0.308392
19	1	0	-1.736665	-0.838222	-2.029687
20	6	0	-2.287192	-2.390565	0.135675
21	7	0	-3.350254	-2.760498	0.481213
22	6	0	0.120689	-2.451558	0.259587
23	7	0	1.142534	-2.834055	0.713163
24	6	0	3.274528	-0.355679	0.713181
25	6	0	3.439436	0.001774	-0.783630
26	1	0	3.347819	-0.901330	-1.390590
27	1	0	4.401950	0.465399	-0.999244
28	1	0	3.487603	-1.398004	0.954790
29	1	0	3.890289	0.270233	1.374012
30	1	0	0.000322	-0.819217	-1.814973

0624aba_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.673478	-0.182039	0.151272
2	6	0	-2.716553	0.684258	0.680538
3	6	0	-1.348515	0.379122	0.670271
4	6	0	-0.992229	-0.854454	0.096510
5	6	0	-1.932276	-1.732520	-0.444895
6	6	0	-3.284028	-1.396466	-0.413290
7	1	0	-4.722673	0.094852	0.177808
8	1	0	-3.030731	1.629657	1.112902
9	1	0	-1.606079	-2.675569	-0.871236
10	1	0	-4.019690	-2.078362	-0.825937
11	7	0	0.396948	-1.256963	0.011143
12	6	0	1.152548	-1.595961	0.997969
13	1	0	0.760716	-1.619541	2.009641
14	6	0	1.124116	-1.271252	-1.298222
15	1	0	0.511809	-1.797363	-2.031131
16	1	0	1.231895	-0.228036	-1.603458
17	6	0	-0.345187	1.376408	1.237511
18	6	0	0.673383	1.913869	0.236449
19	1	0	-0.926601	2.191143	1.686856
20	6	0	0.251952	2.691253	-0.847608
21	7	0	-0.128449	3.341692	-1.752344
22	6	0	2.035287	1.693251	0.434894
23	7	0	3.177959	1.469257	0.627569
24	6	0	2.546015	-1.896380	0.588094
25	6	0	2.452321	-1.969849	-0.956347
26	1	0	2.426534	-3.011240	-1.283117
27	1	0	3.296194	-1.478673	-1.440289
28	1	0	2.918749	-2.805463	1.067139
29	1	0	3.170129	-1.057652	0.928101
30	1	0	0.204415	0.922896	2.069269

0629aaa_Ph_NPiperidin_CHC_CN_CN_PRODUCT_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.703223	-0.952238	-0.079793
2	6	0	-2.501845	-1.645844	0.065079
3	6	0	-1.289371	-0.978533	0.255582
4	6	0	-1.276716	0.437481	0.294970
5	6	0	-2.491758	1.135041	0.138705
6	6	0	-3.685967	0.444144	-0.045981
7	1	0	-4.633431	-1.492114	-0.223395
8	1	0	-2.497017	-2.732308	0.022722
9	1	0	-2.496559	2.218627	0.177527
10	1	0	-4.609492	1.004603	-0.159394
11	7	0	-0.076528	1.113784	0.454942
12	6	0	1.142663	0.425654	0.824072
13	1	0	1.120559	0.096914	1.871168
14	6	0	0.152933	2.503003	0.045584
15	1	0	-0.491233	2.761845	-0.799999
16	1	0	-0.069248	3.201148	0.865066
17	6	0	-0.009097	-1.773322	0.397968
18	6	0	1.247145	-0.930211	0.008488
19	1	0	0.145220	-2.093366	1.434766
20	6	0	2.473029	-1.651960	0.382672
21	7	0	3.435626	-2.210552	0.712046
22	6	0	1.279193	-0.672076	-1.442337
23	7	0	1.292824	-0.463789	-2.583843
24	6	0	2.263611	1.462544	0.601433
25	6	0	1.642279	2.524900	-0.323402
26	1	0	1.767421	2.240691	-1.371731
27	1	0	2.090601	3.511033	-0.183739
28	1	0	3.171650	1.013621	0.190743
29	1	0	2.527935	1.901528	1.567500

30	1	0	-0.047121	-2.679805	-0.211484

0629baa_Ph_NPiperidin_CHC_CN_CN_PRODUCT_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.703306	0.952178	0.079710
2	6	0	-2.501934	1.645815	-0.065021
3	6	0	-1.289427	0.978522	-0.255438
4	6	0	-1.276764	-0.437471	-0.294876
5	6	0	-2.491809	-1.135070	-0.138810
6	6	0	-3.686046	-0.444206	0.045801
7	1	0	-4.633533	1.492027	0.223302
8	1	0	-2.497130	2.732276	-0.022626
9	1	0	-2.496564	-2.218654	-0.177720
10	1	0	-4.609592	-1.004660	0.159065
11	7	0	-0.076521	-1.113761	-0.454684
12	6	0	1.142696	-0.425576	-0.823924
13	1	0	1.120434	-0.096897	-1.871028
14	6	0	0.152929	-2.503042	-0.045559
15	1	0	-0.491154	-2.761986	0.800055
16	1	0	-0.069365	-3.201069	-0.865117
17	6	0	-0.009153	1.773347	-0.397697
18	6	0	1.247176	0.930226	-0.008390
19	6	0	2.472989	1.652023	-0.382773
20	7	0	3.435491	2.210404	-0.712783
21	6	0	1.279364	0.672192	1.442455
22	7	0	1.293191	0.464010	2.583976
23	6	0	2.263632	-1.462501	-0.601390
24	6	0	1.642320	-2.525050	0.323274
25	1	0	1.767607	-2.241101	1.371653
26	1	0	2.090589	-3.511163	0.183310
27	1	0	3.171642	-1.013627	-0.190582
28	1	0	2.528006	-1.901347	-1.567505
29	1	0	0.145113	2.093571	-1.434448
30	1	0	-0.047174	2.679731	0.211902

0631aaa_Ph_NPiperidin_CHC_CN_CN_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.425690	3.234145	-0.106855
2	6	0	-1.795395	1.899097	-0.141091
3	6	0	-0.823911	0.872970	-0.160566
4	6	0	0.563303	1.221221	-0.087630
5	6	0	0.912980	2.582845	-0.080410
6	6	0	-0.066102	3.571007	-0.090372
7	1	0	-2.184035	4.009629	-0.113839
8	1	0	-2.845424	1.641902	-0.210174
9	1	0	1.955967	2.870636	-0.030344
10	1	0	0.232816	4.614686	-0.065990
11	7	0	1.526219	0.199988	-0.042516
12	6	0	1.544889	-0.654897	1.169374
13	1	0	0.519490	-0.845574	1.489667
14	1	0	2.045334	-0.109504	1.988250
15	6	0	2.886969	0.529129	-0.494251
16	1	0	2.813252	1.162138	-1.382098
17	1	0	3.433937	1.097432	0.278149
18	6	0	-1.158378	-0.509348	-0.402855
19	6	0	-2.330860	-1.191157	-0.192846
20	1	0	-0.347458	-1.093856	-0.831658
21	6	0	-2.440170	-2.555963	-0.611912
22	7	0	-2.534092	-3.666868	-0.948396
23	6	0	-3.486273	-0.660311	0.462234
24	7	0	-4.438966	-0.261397	1.000392
25	6	0	2.281646	-1.968000	0.902215
26	1	0	2.310096	-2.552987	1.828216
27	1	0	1.717041	-2.553252	0.165337

28	6	0	3.659657	-0.753255	-0.822558
29	1	0	3.174214	-1.249253	-1.672127
30	1	0	4.673213	-0.483316	-1.139086
31	6	0	3.700127	-1.703559	0.380589
32	1	0	4.300945	-1.249988	1.180830
33	1	0	4.191711	-2.644297	0.110122

0632aba_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.277884	2.805844	-0.183772
2	6	0	-2.231241	1.444752	-0.470724
3	6	0	-1.007364	0.766711	-0.570243
4	6	0	0.178796	1.497982	-0.338216
5	6	0	0.132479	2.862952	-0.032175
6	6	0	-1.093078	3.516017	0.038232
7	1	0	-3.235681	3.313995	-0.137305
8	1	0	-3.150087	0.888761	-0.630178
9	1	0	1.058417	3.403037	0.135475
10	1	0	-1.125325	4.577598	0.261077
11	7	0	1.419890	0.793299	-0.338995
12	6	0	1.470946	-0.231519	-1.245511
13	1	0	1.156578	0.067719	-2.246202
14	6	0	2.081726	0.664966	0.985971
15	1	0	2.263510	1.676396	1.355688
16	1	0	1.381079	0.180071	1.681112
17	6	0	-0.995021	-0.710907	-0.860181
18	6	0	-1.600490	-1.598974	0.102965
19	1	0	-1.255787	-0.954087	-1.893105
20	6	0	-1.540693	-1.314119	1.484879
21	7	0	-1.471005	-1.063489	2.626807
22	6	0	-2.101189	-2.858052	-0.295539
23	7	0	-2.524218	-3.894518	-0.638376
24	6	0	2.589606	-1.244502	-1.197291
25	1	0	2.246979	-2.170844	-1.668649
26	1	0	3.390286	-0.855044	-1.842433
27	6	0	3.378262	-0.133517	0.898661
28	1	0	4.129185	0.437035	0.338894
29	1	0	3.763795	-0.269645	1.913511
30	6	0	3.128725	-1.481488	0.215918
31	1	0	2.407393	-2.064878	0.801162
32	1	0	4.049511	-2.069295	0.162704
33	1	0	0.265984	-0.924737	-0.975637

0634aaa_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.432278	2.685278	0.209783
2	6	0	-2.375657	1.468053	-0.467480
3	6	0	-1.193448	0.716700	-0.544180
4	6	0	-0.067333	1.259756	0.094592
5	6	0	-0.100769	2.478120	0.775247
6	6	0	-1.294116	3.194542	0.837482
7	1	0	-3.365996	3.237746	0.245941
8	1	0	-3.268261	1.078266	-0.948073
9	1	0	0.801310	2.855670	1.245870
10	1	0	-1.329601	4.140153	1.367757
11	7	0	1.220045	0.573577	0.032485
12	6	0	1.614746	-0.184026	1.002881
13	1	0	0.909204	-0.338348	1.812616
14	6	0	2.072924	0.877241	-1.157718
15	1	0	1.402539	0.896035	-2.018511
16	1	0	2.451665	1.893563	-1.009782
17	6	0	-1.196918	-0.640474	-1.236020
18	6	0	-1.567445	-1.801124	-0.313239
19	1	0	-1.911430	-0.594425	-2.064284

20	6	0	-2.909220	-2.106239	-0.071874
21	7	0	-4.047422	-2.353742	0.103584
22	6	0	-0.572246	-2.454035	0.408655
23	7	0	0.309347	-2.975127	0.996559
24	6	0	2.942507	-0.844034	1.064431
25	1	0	3.323282	-0.712302	2.084134
26	1	0	2.725554	-1.918203	0.974055
27	6	0	3.199998	-0.135139	-1.327319
28	1	0	2.789711	-1.082563	-1.694752
29	1	0	3.880421	0.242576	-2.095232
30	6	0	3.931076	-0.357469	-0.000305
31	1	0	4.395094	0.578892	0.328549
32	1	0	4.732693	-1.090210	-0.118065
33	1	0	-0.220902	-0.842695	-1.688233

0634aba_Ph_NPiperidin_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.735242	0.880336	0.155269
2	6	0	2.982881	-0.166171	0.689368
3	6	0	1.581279	-0.156744	0.675547
4	6	0	0.971916	0.967233	0.092064
5	6	0	1.704710	2.024704	-0.446802
6	6	0	3.097529	1.982343	-0.413651
7	1	0	4.819253	0.832705	0.183517
8	1	0	3.488716	-1.020701	1.129018
9	1	0	1.187438	2.877706	-0.874447
10	1	0	3.672401	2.804178	-0.826757
11	7	0	-0.482072	1.064848	0.018917
12	6	0	-1.174022	1.331009	1.076142
13	1	0	-0.609180	1.495807	1.990573
14	6	0	-1.105785	0.873247	-1.328391
15	1	0	-0.437485	1.358616	-2.041151
16	1	0	-1.078980	-0.203503	-1.513750
17	6	0	0.807088	-1.334315	1.252600
18	6	0	-0.025077	-2.112659	0.238102
19	1	0	1.537859	-1.981388	1.754719
20	6	0	0.597094	-2.741946	-0.845825
21	7	0	1.144091	-3.257498	-1.752072
22	6	0	-1.392845	-2.291846	0.437964
23	7	0	-2.552271	-2.411867	0.621977
24	6	0	-2.653845	1.436364	1.111806
25	1	0	-2.995205	0.869869	1.986765
26	1	0	-2.870017	2.488365	1.354037
27	6	0	-2.517728	1.444820	-1.389197
28	1	0	-2.468698	2.539248	-1.423977
29	1	0	-2.973656	1.111566	-2.325479
30	6	0	-3.341492	0.988456	-0.181644
31	1	0	-3.425142	-0.103390	-0.178484
32	1	0	-4.351597	1.402958	-0.221578
33	1	0	0.134391	-0.989389	2.045120

0639baa_Ph_NPiperidin_CHC_CN_CN_PRODUCT_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.996602	-0.523807	0.024040
2	6	0	2.901201	-1.380241	0.005620
3	6	0	1.593537	-0.894895	-0.139715
4	6	0	1.383945	0.492615	-0.276948
5	6	0	2.499290	1.352681	-0.259566
6	6	0	3.786768	0.852876	-0.108432
7	1	0	4.999705	-0.921527	0.139883
8	1	0	3.050896	-2.451484	0.114825
9	1	0	2.350419	2.419290	-0.388466
10	1	0	4.629140	1.538119	-0.105041
11	7	0	0.080879	1.030225	-0.438110

12	6	0	-0.930956	0.087013	-0.877761
13	1	0	-0.596142	-0.323996	-1.837175
14	6	0	-0.301563	2.094452	0.523191
15	1	0	-0.378311	1.689022	1.542013
16	1	0	0.503067	2.830745	0.536079
17	6	0	0.455106	-1.892534	-0.159769
18	6	0	-0.939320	-1.224148	0.051558
19	6	0	-1.990163	-2.160472	-0.376136
20	7	0	-2.807890	-2.895658	-0.748923
21	6	0	-1.160077	-0.922012	1.477119
22	7	0	-1.319282	-0.718817	2.609014
23	6	0	-2.300073	0.743102	-1.119505
24	6	0	-1.613080	2.776425	0.143279
25	1	0	-1.867567	3.498862	0.925844
26	1	0	-1.478187	3.338258	-0.789570
27	1	0	-3.051744	-0.038635	-1.262018
28	1	0	-2.224513	1.277303	-2.073679
29	1	0	0.412776	-2.397783	-1.131184
30	1	0	0.610805	-2.671413	0.591491
31	6	0	-2.723842	1.740930	-0.038825
32	1	0	-2.919354	1.229447	0.911438
33	1	0	-3.661193	2.221632	-0.337190

0641aaa_Ph_NMorf_CHC_CN_CN_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.356793	3.249818	-0.110564
2	6	0	-1.755943	1.922765	-0.148464
3	6	0	-0.807355	0.876316	-0.172396
4	6	0	0.585052	1.196304	-0.102231
5	6	0	0.966347	2.547536	-0.089738
6	6	0	0.008870	3.557709	-0.095219
7	1	0	-2.098503	4.041217	-0.114193
8	1	0	-2.811353	1.688843	-0.217292
9	1	0	2.015697	2.811907	-0.042991
10	1	0	0.330557	4.594435	-0.069365
11	7	0	1.527561	0.151507	-0.063957
12	6	0	1.550243	-0.695291	1.149582
13	1	0	0.532551	-0.952592	1.448174
14	1	0	2.019083	-0.145043	1.981343
15	6	0	2.896985	0.452413	-0.500783
16	1	0	2.861697	1.028556	-1.429216
17	1	0	3.444703	1.040586	0.253366
18	6	0	-1.173646	-0.499413	-0.414637
19	6	0	-2.356942	-1.154965	-0.188675
20	1	0	-0.382424	-1.100167	-0.857147
21	6	0	-2.502925	-2.516698	-0.607665
22	7	0	-2.627047	-3.624485	-0.944090
23	6	0	-3.490674	-0.599014	0.484067
24	7	0	-4.426070	-0.180371	1.037034
25	6	0	2.346065	-1.966519	0.873160
26	1	0	2.442980	-2.555537	1.788898
27	1	0	1.827123	-2.574649	0.115721
28	6	0	3.641700	-0.859724	-0.739774
29	1	0	3.163652	-1.409426	-1.565174
30	1	0	4.682096	-0.657820	-1.007236
31	8	0	3.668141	-1.663036	0.436527

0643abb_Ph_NMorf_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.998571	2.999368	-0.192997
2	6	0	-2.079719	1.642050	-0.490666
3	6	0	-0.925954	0.849803	-0.578898
4	6	0	0.318282	1.465825	-0.326017
5	6	0	0.403456	2.824897	-0.006041

6	6	0	-0.754998	3.591590	0.053432
7	1	0	-2.903559	3.597066	-0.155251
8	1	0	-3.045647	1.177973	-0.664804
9	1	0	1.375084	3.270009	0.180693
10	1	0	-0.689400	4.649225	0.286863
11	7	0	1.485667	0.642862	-0.320650
12	6	0	1.472413	-0.366075	-1.231844
13	1	0	1.213751	-0.064321	-2.246493
14	6	0	2.132508	0.422991	0.995086
15	1	0	2.456934	1.391374	1.382851
16	1	0	1.395240	0.001510	1.690476
17	6	0	-1.046749	-0.624683	-0.870478
18	6	0	-1.738232	-1.445516	0.103307
19	1	0	-1.355373	-0.833404	-1.898082
20	6	0	-2.379789	-2.639763	-0.288621
21	7	0	-2.920876	-3.621994	-0.626246
22	6	0	-1.624287	-1.170498	1.482640
23	7	0	-1.505501	-0.925587	2.622188
24	6	0	2.498468	-1.470259	-1.123742
25	1	0	2.096574	-2.396850	-1.540728
26	1	0	3.362688	-1.175087	-1.744593
27	6	0	3.314994	-0.522169	0.844429
28	1	0	4.123550	-0.048693	0.269529
29	1	0	3.697880	-0.795802	1.829094
30	8	0	2.893874	-1.727691	0.206290
31	1	0	0.155324	-0.963816	-0.984456

0644aaa_Ph_NMorf_CHC_CN_CN_BZW_3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.519496	2.622585	0.183646
2	6	0	-2.428004	1.406533	-0.492409
3	6	0	-1.227314	0.685026	-0.562526
4	6	0	-0.119877	1.258458	0.083138
5	6	0	-0.186854	2.475976	0.762320
6	6	0	-1.398709	3.161506	0.816971
7	1	0	-3.467511	3.150359	0.214492
8	1	0	-3.307801	0.994022	-0.977471
9	1	0	0.702554	2.877421	1.237030
10	1	0	-1.461211	4.106122	1.346344
11	7	0	1.186747	0.607538	0.032245
12	6	0	1.614996	-0.130431	1.000409
13	1	0	0.942558	-0.334062	1.826160
14	6	0	2.054274	0.909508	-1.142678
15	1	0	1.419454	0.892856	-2.029913
16	1	0	2.436330	1.924572	-1.006941
17	6	0	-1.194081	-0.673108	-1.251846
18	6	0	-1.472118	-1.846508	-0.313092
19	1	0	-1.941714	-0.661964	-2.051386
20	6	0	-2.787358	-2.204082	-0.004294
21	7	0	-3.904294	-2.496238	0.227437
22	6	0	-0.416005	-2.451065	0.360114
23	7	0	0.521356	-2.920522	0.904553
24	6	0	2.988165	-0.710997	1.023473
25	1	0	3.434336	-0.487707	1.999083
26	1	0	2.857627	-1.804121	0.964802
27	6	0	3.180052	-0.111148	-1.233504
28	1	0	2.792508	-1.091423	-1.542686
29	1	0	3.918622	0.219763	-1.964652
30	8	0	3.843802	-0.205413	0.025063
31	1	0	-0.228862	-0.831502	-1.743349

0644aba_Ph_NMorf_CHC_CN_CN_BZW_3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.420496	2.649704	-0.140369

2	6	0	2.361479	1.417699	0.505186
3	6	0	1.168865	0.680619	0.600166
4	6	0	0.033029	1.269520	0.020734
5	6	0	0.070322	2.501860	-0.637718
6	6	0	1.272292	3.197396	-0.718294
7	1	0	3.362696	3.186289	-0.190268
8	1	0	3.260931	0.999310	0.946646
9	1	0	-0.838655	2.917250	-1.060797
10	1	0	1.307177	4.159724	-1.217290
11	7	0	-1.262607	0.600694	0.080488
12	6	0	-1.930705	0.539317	1.180678
13	1	0	-1.518673	1.034487	2.055613
14	6	0	-1.805007	0.000471	-1.173826
15	1	0	-1.539008	0.671808	-1.991831
16	1	0	-1.300704	-0.960759	-1.316102
17	6	0	1.200963	-0.702964	1.238840
18	6	0	1.606740	-1.807398	0.263282
19	1	0	1.909457	-0.667134	2.073366
20	6	0	2.952087	-1.987602	-0.067739
21	7	0	4.094682	-2.126994	-0.318205
22	6	0	0.630185	-2.536760	-0.410429
23	7	0	-0.229307	-3.131717	-0.958801
24	6	0	-3.245126	-0.152365	1.293500
25	1	0	-3.193332	-0.846347	2.140738
26	1	0	-3.983977	0.622493	1.566979
27	6	0	-3.312062	-0.166073	-1.049154
28	1	0	-3.815997	0.809940	-1.060087
29	1	0	-3.686153	-0.764143	-1.880722
30	8	0	-3.619809	-0.877244	0.150260
31	1	0	0.233989	-0.959400	1.678151

0649aba_Ph_NMorf_CHC_CN_CN_PR_3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.976713	-0.587317	0.051756
2	6	0	2.865464	-1.423600	0.032106
3	6	0	1.569773	-0.914977	-0.136530
4	6	0	1.393114	0.473480	-0.297962
5	6	0	2.521167	1.314101	-0.276266
6	6	0	3.796827	0.791237	-0.101260
7	1	0	4.970206	-1.002858	0.186066
8	1	0	2.993242	-2.495541	0.159418
9	1	0	2.391921	2.381710	-0.418260
10	1	0	4.652587	1.459471	-0.094288
11	7	0	0.102037	1.037714	-0.477615
12	6	0	-0.936066	0.111547	-0.889134
13	1	0	-0.661403	-0.296037	-1.869411
14	6	0	-0.270770	2.096883	0.488976
15	1	0	-0.272371	1.711616	1.516516
16	1	0	0.473849	2.893978	0.436736
17	6	0	0.408747	-1.886164	-0.155167
18	6	0	-0.970673	-1.183585	0.044979
19	6	0	-2.043638	-2.097533	-0.379376
20	7	0	-2.881146	-2.810051	-0.751666
21	6	0	-1.193753	-0.856844	1.465621
22	7	0	-1.347742	-0.648087	2.596823
23	6	0	-2.282237	0.823093	-1.063668
24	6	0	-1.635694	2.682316	0.161648
25	1	0	-1.962348	3.339958	0.970150
26	1	0	-1.594427	3.262406	-0.772365
27	1	0	-3.087039	0.094099	-1.179803
28	1	0	-2.227666	1.423948	-1.983583
29	1	0	0.359395	-2.397577	-1.123003
30	1	0	0.541681	-2.662065	0.603304
31	8	0	-2.610439	1.646755	0.040175

0651aaa_Ph_NMeEt_CHC_CN_CN_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.079277	-3.034042	-0.089187
2	6	0	0.004440	-2.172416	-0.113155
3	6	0	-0.175199	-0.770809	-0.167163
4	6	0	-1.503284	-0.232421	-0.131833
5	6	0	-2.587037	-1.130836	-0.142720
6	6	0	-2.376504	-2.504626	-0.120557
7	1	0	-0.923103	-4.107172	-0.070491
8	1	0	1.006547	-2.582137	-0.149924
9	1	0	-3.601532	-0.752663	-0.128869
10	1	0	-3.233687	-3.171183	-0.107952
11	7	0	-1.689930	1.156442	-0.108972
12	6	0	-1.137356	1.911308	1.042966
13	1	0	-0.339205	1.316239	1.489675
14	1	0	-1.923572	2.007120	1.808518
15	6	0	-2.995722	1.658413	-0.535277
16	1	0	-2.915640	2.727133	-0.741684
17	1	0	-3.306177	1.161422	-1.455947
18	1	0	-3.776710	1.519723	0.228021
19	6	0	0.916579	0.135944	-0.418686
20	6	0	2.263081	-0.001718	-0.186131
21	1	0	0.620673	1.071881	-0.885970
22	6	0	3.163828	1.019197	-0.628753
23	7	0	3.900084	1.848634	-0.984277
24	6	0	2.870115	-1.089455	0.516001
25	7	0	3.393539	-1.955530	1.092679
26	6	0	-0.604089	3.295472	0.678706
27	1	0	-1.383146	3.943463	0.267715
28	1	0	-0.214839	3.781749	1.578518
29	1	0	0.207093	3.233542	-0.052874

0653aaa_Ph_NMeEt_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.524950	-2.795772	-0.438479
2	6	0	-0.374524	-2.033048	-0.648960
3	6	0	-0.361843	-0.657326	-0.399345
4	6	0	-1.554932	-0.054670	0.054361
5	6	0	-2.705310	-0.813380	0.269870
6	6	0	-2.691495	-2.185881	0.022158
7	1	0	-1.502728	-3.864701	-0.624488
8	1	0	0.534265	-2.506221	-1.007574
9	1	0	-3.602830	-0.327238	0.638097
10	1	0	-3.586890	-2.773330	0.196976
11	7	0	-1.581052	1.371200	0.241099
12	6	0	-0.399768	1.885610	0.694319
13	1	0	-0.005554	1.354723	1.563555
14	6	0	-2.418669	2.139527	-0.693375
15	1	0	-2.594705	3.138264	-0.293770
16	1	0	-1.956833	2.217847	-1.685519
17	1	0	-3.377604	1.632668	-0.794356
18	6	0	0.887783	0.150975	-0.673986
19	6	0	2.151148	-0.299524	-0.131388
20	1	0	0.973877	0.470908	-1.717323
21	6	0	3.362145	0.139037	-0.710200
22	7	0	4.361702	0.496529	-1.204778
23	6	0	2.233224	-1.038356	1.069792
24	7	0	2.311302	-1.660520	2.059088
25	6	0	-0.104449	3.354657	0.634374
26	1	0	-0.258289	3.773394	-0.361900
27	1	0	-0.754652	3.889758	1.338122
28	1	0	0.929027	3.530655	0.938233
29	1	0	0.569096	1.261718	-0.152752

0654aaa_Ph_NMeEt_CHC_CN_CN_ZW_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.451320	-3.214691	0.433482
2	6	0	1.038985	-2.163264	-0.266924
3	6	0	0.352636	-0.965319	-0.519188
4	6	0	-0.960078	-0.886215	-0.030422
5	6	0	-1.570558	-1.927712	0.670640
6	6	0	-0.856840	-3.099668	0.909057
7	1	0	1.014170	-4.126497	0.607110
8	1	0	2.058801	-2.260357	-0.627616
9	1	0	-2.591210	-1.815696	1.021953
10	1	0	-1.320681	-3.912644	1.457243
11	7	0	-1.769856	0.307652	-0.285459
12	6	0	-1.819198	1.248439	0.601633
13	1	0	-1.198234	1.088293	1.477416
14	6	0	-2.536103	0.281092	-1.548887
15	1	0	-3.004287	1.241329	-1.742903
16	1	0	-1.849833	0.032593	-2.358404
17	1	0	-3.295010	-0.499733	-1.471406
18	6	0	1.057530	0.180087	-1.234825
19	6	0	1.890927	1.063296	-0.306671
20	1	0	1.709603	-0.249975	-2.001698
21	6	0	3.214531	0.726865	-0.013385
22	7	0	4.333429	0.430867	0.206078
23	6	0	1.278682	2.113524	0.371905
24	7	0	0.708081	2.990924	0.918582
25	6	0	-2.607669	2.496535	0.558693
26	1	0	-3.217999	2.632591	-0.330669
27	1	0	-3.247306	2.520591	1.448842
28	1	0	-1.895886	3.323014	0.661901
29	1	0	0.331295	0.802563	-1.766837

0659aba_Ph_NMeEt_CHC_CN_CN_PR_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.489048	-1.268030	-0.073758
2	6	0	2.197415	-1.781974	-0.173700
3	6	0	1.076020	-0.949749	-0.207461
4	6	0	1.238987	0.454274	-0.122608
5	6	0	2.550900	0.965677	-0.028515
6	6	0	3.653746	0.115117	-0.002816
7	1	0	4.345713	-1.933608	-0.051526
8	1	0	2.046211	-2.857314	-0.228236
9	1	0	2.718312	2.033608	0.015785
10	1	0	4.648477	0.545383	0.068832
11	7	0	0.117436	1.297877	-0.089200
12	6	0	-1.119912	0.796981	-0.686244
13	1	0	-0.969250	0.544026	-1.747122
14	6	0	0.343208	2.734607	0.023782
15	1	0	1.009097	2.932299	0.867108
16	1	0	0.790360	3.172044	-0.881084
17	6	0	-0.289621	-1.580531	-0.350777
18	6	0	-1.433940	-0.590788	0.012883
19	6	0	-2.711541	-1.151176	-0.463249
20	7	0	-3.700956	-1.605432	-0.864750
21	6	0	-1.529452	-0.399856	1.474196
22	7	0	-1.607110	-0.256156	2.622755
23	6	0	-2.299580	1.761597	-0.586661
24	1	0	-3.191834	1.283369	-0.996349
25	1	0	-2.119786	2.663114	-1.174600
26	1	0	-0.462576	-1.890324	-1.387424
27	1	0	-0.373421	-2.480696	0.264340
28	1	0	-0.591772	3.248027	0.229958
29	1	0	-2.506789	2.049155	0.448258

0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.092606	-1.270762	0.050132
2	6	0	3.301606	-0.133861	-0.027387
3	6	0	1.900672	-0.221376	-0.168205
4	6	0	1.283428	-1.512172	-0.182745
5	6	0	2.107277	-2.648037	-0.124670
6	6	0	3.489606	-2.529184	-0.013012
7	1	0	5.169695	-1.178107	0.139862
8	1	0	3.774579	0.840367	-0.024784
9	1	0	1.663671	-3.635888	-0.137705
10	1	0	4.097240	-3.427804	0.041746
11	7	0	-0.121607	-1.622212	-0.276023
12	6	0	-0.908062	-1.074498	0.844726
13	1	0	-0.344147	-0.246400	1.283338
14	1	0	-1.000478	-1.833496	1.640493
15	6	0	-0.654277	-2.900026	-0.744822
16	1	0	-1.708952	-2.767016	-0.993090
17	1	0	-0.125278	-3.218003	-1.645495
18	1	0	-0.584864	-3.699241	0.011111
19	6	0	-2.296545	-0.587261	0.464350
20	6	0	-3.290254	-0.538850	1.450511
21	6	0	-2.605833	-0.134062	-0.823203
22	6	0	-4.557046	-0.032642	1.163278
23	1	0	-3.068247	-0.897429	2.453053
24	6	0	-3.875938	0.366904	-1.114970
25	1	0	-1.853471	-0.189890	-1.603948
26	6	0	-4.853987	0.423355	-0.122479
27	1	0	-5.313606	0.000381	1.941799
28	1	0	-4.098124	0.714790	-2.119427
29	1	0	-5.840891	0.815280	-0.349073
30	6	0	1.078733	0.944149	-0.428995
31	6	0	1.298493	2.264683	-0.146198
32	1	0	0.144732	0.733446	-0.941796
33	6	0	0.356854	3.248940	-0.596219
34	7	0	-0.407063	4.046182	-0.963720
35	6	0	2.410221	2.770308	0.602586
36	7	0	3.303357	3.201083	1.212292

0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMacn.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.181593	-0.900135	-0.051828
2	6	0	3.262962	0.134671	-0.089162
3	6	0	1.872038	-0.114299	-0.153920
4	6	0	1.402942	-1.469795	-0.119432
5	6	0	2.359748	-2.503256	-0.111327
6	6	0	3.720318	-2.222443	-0.078309
7	1	0	5.244572	-0.686610	-0.026182
8	1	0	3.620181	1.156320	-0.128699
9	1	0	2.037467	-3.536284	-0.093369
10	1	0	4.429027	-3.044832	-0.054579
11	7	0	0.030483	-1.750468	-0.117841
12	6	0	-0.812271	-1.172804	0.943225
13	1	0	-0.279179	-0.331264	1.393061
14	1	0	-0.935425	-1.914235	1.748464
15	6	0	-0.384545	-3.108327	-0.473986
16	1	0	-1.459711	-3.102457	-0.661247
17	1	0	0.119303	-3.430220	-1.386965
18	1	0	-0.182543	-3.836658	0.325371
19	6	0	-2.188066	-0.710319	0.486962
20	6	0	-3.165344	-0.452942	1.459419
21	6	0	-2.507988	-0.499913	-0.858985
22	6	0	-4.426274	0.017963	1.096282
23	1	0	-2.934835	-0.621329	2.508722
24	6	0	-3.774084	-0.033288	-1.225701
25	1	0	-1.768391	-0.715497	-1.624072
26	6	0	-4.735623	0.230280	-0.250589
27	1	0	-5.169506	0.214443	1.863500
28	1	0	-4.005517	0.120663	-2.275640

29	1	0	-5.718993	0.592514	-0.534937
30	6	0	0.923556	0.942822	-0.404117
31	6	0	1.011825	2.292931	-0.167525
32	1	0	-0.003971	0.624787	-0.871676
33	6	0	-0.041787	3.156978	-0.607489
34	7	0	-0.894560	3.866866	-0.961028
35	6	0	2.074607	2.942178	0.535399
36	7	0	2.916344	3.502008	1.113831

0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMdce.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.173186	-0.945784	-0.042436
2	6	0	3.268882	0.101909	-0.084913
3	6	0	1.875542	-0.127853	-0.156705
4	6	0	1.388134	-1.476421	-0.126039
5	6	0	2.329857	-2.522866	-0.111553
6	6	0	3.694388	-2.261217	-0.071020
7	1	0	5.238778	-0.746485	-0.010727
8	1	0	3.640394	1.118538	-0.121600
9	1	0	1.992846	-3.551294	-0.095738
10	1	0	4.391532	-3.093355	-0.043351
11	7	0	0.010301	-1.736971	-0.134855
12	6	0	-0.824598	-1.159016	0.932536
13	1	0	-0.287288	-0.317696	1.377850
14	1	0	-0.943543	-1.899791	1.739405
15	6	0	-0.419980	-3.087423	-0.499808
16	1	0	-1.493799	-3.067022	-0.693781
17	1	0	0.085817	-3.411544	-1.410994
18	1	0	-0.232681	-3.822610	0.297237
19	6	0	-2.202248	-0.694550	0.484550
20	6	0	-3.180241	-0.456176	1.460799
21	6	0	-2.522221	-0.461592	-0.857641
22	6	0	-4.441861	0.018732	1.105520
23	1	0	-2.949774	-0.642215	2.507152
24	6	0	-3.788869	0.008782	-1.216574
25	1	0	-1.782056	-0.663024	-1.626023
26	6	0	-4.751022	0.253830	-0.237331
27	1	0	-5.185641	0.200680	1.875775
28	1	0	-4.020231	0.180983	-2.263671
29	1	0	-5.734767	0.619628	-0.515694
30	6	0	0.941668	0.943308	-0.408578
31	6	0	1.046825	2.290300	-0.165385
32	1	0	0.012832	0.638930	-0.882683
33	6	0	0.008376	3.171529	-0.608606
34	7	0	-0.831277	3.894898	-0.965737
35	6	0	2.115785	2.920937	0.545875
36	7	0	2.963542	3.464601	1.130693

0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMtol.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.126140	-1.155942	0.015769
2	6	0	3.292916	-0.050171	-0.048128
3	6	0	1.892305	-0.189281	-0.163091
4	6	0	1.320347	-1.502514	-0.161229
5	6	0	2.188550	-2.607507	-0.120183
6	6	0	3.566519	-2.436463	-0.034917
7	1	0	5.200710	-1.024937	0.083400
8	1	0	3.730335	0.940431	-0.061585
9	1	0	1.783301	-3.611509	-0.122691
10	1	0	4.207428	-3.312085	0.009613
11	7	0	-0.076587	-1.667123	-0.223294
12	6	0	-0.879541	-1.103751	0.877471
13	1	0	-0.324267	-0.270402	1.316456
14	1	0	-0.982037	-1.853895	1.679264

15	6	0	-0.575089	-2.973904	-0.651520
16	1	0	-1.638225	-2.881266	-0.880608
17	1	0	-0.055593	-3.296229	-1.555864
18	1	0	-0.462609	-3.749184	0.122524
19	6	0	-2.264140	-0.624214	0.471804
20	6	0	-3.251513	-0.504175	1.459100
21	6	0	-2.578415	-0.253638	-0.840663
22	6	0	-4.516755	-0.008964	1.146686
23	1	0	-3.025692	-0.798370	2.481457
24	6	0	-3.847631	0.236658	-1.157229
25	1	0	-1.831751	-0.365638	-1.620894
26	6	0	-4.819282	0.364308	-0.164991
27	1	0	-5.268119	0.080115	1.925843
28	1	0	-4.074170	0.518232	-2.181354
29	1	0	-5.805321	0.746743	-0.410834
30	6	0	1.030090	0.942917	-0.422719
31	6	0	1.209628	2.274773	-0.154518
32	1	0	0.097603	0.698704	-0.923629
33	6	0	0.236432	3.224556	-0.608100
34	7	0	-0.550421	3.999140	-0.976593
35	6	0	2.303340	2.826020	0.586761
36	7	0	3.176293	3.300418	1.193755

0661aaa_Ph_NMeBn_CHC_CN_CN_B3lyp631pd_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.183273	-0.892066	-0.052827
2	6	0	3.262287	0.140567	-0.089423
3	6	0	1.871813	-0.111714	-0.153541
4	6	0	1.405820	-1.468393	-0.118834
5	6	0	2.365119	-2.499643	-0.111671
6	6	0	3.724968	-2.215541	-0.079336
7	1	0	5.245792	-0.676197	-0.027847
8	1	0	3.617098	1.163048	-0.129243
9	1	0	2.045354	-3.533442	-0.093701
10	1	0	4.435627	-3.036244	-0.056108
11	7	0	0.034262	-1.752329	-0.116036
12	6	0	-0.809816	-1.175511	0.944444
13	1	0	-0.277606	-0.334020	1.395399
14	1	0	-0.933394	-1.917500	1.749003
15	6	0	-0.377997	-3.111316	-0.471487
16	1	0	-1.453261	-3.107810	-0.658241
17	1	0	0.126066	-3.432437	-1.384594
18	1	0	-0.173981	-3.838729	0.328095
19	6	0	-2.185452	-0.713407	0.487210
20	6	0	-3.162628	-0.453752	1.459247
21	6	0	-2.505533	-0.505911	-0.859180
22	6	0	-4.423571	0.016517	1.095210
23	1	0	-2.932039	-0.619960	2.508868
24	6	0	-3.771641	-0.039849	-1.226788
25	1	0	-1.766152	-0.723395	-1.623934
26	6	0	-4.733084	0.225964	-0.252137
27	1	0	-5.166723	0.214642	1.862087
28	1	0	-4.003217	0.111610	-2.277065
29	1	0	-5.716504	0.587544	-0.537166
30	6	0	0.920827	0.942819	-0.403560
31	6	0	1.005698	2.293475	-0.167806
32	1	0	-0.006236	0.622226	-0.870244
33	6	0	-0.050898	3.154068	-0.607007
34	7	0	-0.906500	3.861101	-0.959563
35	6	0	2.066833	2.946201	0.534186
36	7	0	2.906963	3.509172	1.111955

0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMacn_TS_HC.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	4.158161	-1.071979	-0.154824
2	6	0	3.268317	-0.042488	-0.467958
3	6	0	1.885737	-0.223580	-0.366653
4	6	0	1.404376	-1.487404	0.041667
5	6	0	2.293055	-2.515240	0.361649
6	6	0	3.668979	-2.309579	0.260829
7	1	0	5.227263	-0.899906	-0.225523
8	1	0	3.645321	0.921631	-0.794650
9	1	0	1.904801	-3.470495	0.699123
10	1	0	4.352193	-3.112906	0.516644
11	7	0	-0.011441	-1.713989	0.089178
12	6	0	-0.730819	-0.596093	0.465007
13	1	0	-0.350645	-0.164622	1.394831
14	6	0	-0.544841	-2.738753	-0.816052
15	1	0	-1.582620	-2.946217	-0.557904
16	1	0	-0.482183	-2.440839	-1.869866
17	1	0	0.034890	-3.652412	-0.682964
18	6	0	-2.192943	-0.449477	0.299910
19	6	0	-2.939985	-0.046761	1.421897
20	6	0	-2.852837	-0.617429	-0.932266
21	6	0	-4.317005	0.143184	1.325672
22	1	0	-2.437952	0.104720	2.372828
23	6	0	-4.227386	-0.417365	-1.025782
24	1	0	-2.290746	-0.878501	-1.821888
25	6	0	-4.963856	-0.043622	0.102410
26	1	0	-4.882086	0.441542	2.202910
27	1	0	-4.723929	-0.545327	-1.982318
28	1	0	-6.035533	0.110669	0.024396
29	6	0	0.946930	0.894444	-0.756285
30	6	0	1.154212	2.217836	-0.230501
31	1	0	0.683881	0.898551	-1.818851
32	6	0	0.586377	3.334819	-0.885596
33	7	0	0.124872	4.255839	-1.440916
34	6	0	1.775896	2.446997	1.019116
35	7	0	2.296550	2.650717	2.047402
36	1	0	-0.166730	0.421084	-0.299868

0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdce_TS_HC.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.159107	-1.066636	-0.142366
2	6	0	3.268928	-0.037883	-0.456292
3	6	0	1.886273	-0.222157	-0.363564
4	6	0	1.406160	-1.488056	0.038310
5	6	0	2.294772	-2.515784	0.358798
6	6	0	3.670627	-2.307055	0.265598
7	1	0	5.228209	-0.891739	-0.205825
8	1	0	3.645257	0.928833	-0.775914
9	1	0	1.906587	-3.472725	0.691759
10	1	0	4.354389	-3.109721	0.522129
11	7	0	-0.010162	-1.716770	0.080909
12	6	0	-0.732492	-0.605091	0.464279
13	1	0	-0.348113	-0.172240	1.391437
14	6	0	-0.540312	-2.741344	-0.825452
15	1	0	-1.577477	-2.952795	-0.567876
16	1	0	-0.478527	-2.442100	-1.879159
17	1	0	0.042567	-3.653348	-0.694504
18	6	0	-2.192962	-0.455568	0.300735
19	6	0	-2.934803	-0.036832	1.420676
20	6	0	-2.858630	-0.633557	-0.927231
21	6	0	-4.310981	0.158714	1.327215
22	1	0	-2.428699	0.123298	2.368039
23	6	0	-4.232359	-0.428046	-1.017978
24	1	0	-2.301556	-0.905496	-1.816733
25	6	0	-4.963113	-0.038562	0.108526
26	1	0	-4.871314	0.469985	2.202996
27	1	0	-4.732833	-0.563231	-1.971484
28	1	0	-6.034236	0.120380	0.032428
29	6	0	0.945691	0.894794	-0.755426
30	6	0	1.154624	2.220718	-0.233219
31	1	0	0.692185	0.899557	-1.820586

32	6	0	0.593235	3.335155	-0.898211
33	7	0	0.136021	4.251234	-1.464996
34	6	0	1.764050	2.450266	1.022348
35	7	0	2.273977	2.650609	2.056566
36	1	0	-0.162176	0.427372	-0.304534

0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMtol_TS_HC_f2.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.499643	-3.183831	0.330181
2	6	0	2.073541	-1.921509	0.325695
3	6	0	1.436922	-0.832588	-0.308960
4	6	0	0.148969	-1.027009	-0.901456
5	6	0	-0.397622	-2.321194	-0.910730
6	6	0	0.269030	-3.382202	-0.305930
7	1	0	2.013938	-4.012654	0.804728
8	1	0	3.051408	-1.782242	0.770391
9	1	0	-1.367508	-2.490316	-1.362767
10	1	0	-0.185013	-4.368741	-0.313431
11	7	0	-0.516842	0.067853	-1.482394
12	6	0	-0.939792	1.183013	-0.595446
13	1	0	-0.141023	1.366022	0.125350
14	6	0	-1.475971	-0.218780	-2.547339
15	1	0	-2.434689	-0.618171	-2.188311
16	1	0	-1.683301	0.711690	-3.084318
17	1	0	-1.037558	-0.929217	-3.251236
18	6	0	-2.248222	0.947510	0.140411
19	6	0	-2.292341	0.121350	1.273460
20	6	0	-3.435673	1.544051	-0.301802
21	6	0	-3.495090	-0.106392	1.941589
22	1	0	-1.378732	-0.339155	1.639130
23	6	0	-4.641541	1.319614	0.365637
24	1	0	-3.414416	2.197018	-1.171063
25	6	0	-4.673720	0.491446	1.488098
26	1	0	-3.511624	-0.743914	2.820733
27	1	0	-5.552058	1.793876	0.011162
28	1	0	-5.609351	0.317364	2.011213
29	6	0	2.095123	0.437736	-0.519852
30	6	0	3.116411	1.034571	0.171841
31	1	0	1.721572	0.995428	-1.375665
32	6	0	3.659716	2.273147	-0.302346
33	7	0	4.096277	3.281012	-0.688066
34	6	0	3.689376	0.532395	1.383716
35	7	0	4.166203	0.147678	2.373743
36	1	0	-1.023663	2.079245	-1.219511

0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMw_TS_HC.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.157999	-1.073113	-0.158667
2	6	0	3.268114	-0.043470	-0.471349
3	6	0	1.885601	-0.223753	-0.367427
4	6	0	1.404024	-1.487020	0.042734
5	6	0	2.292869	-2.514900	0.362196
6	6	0	3.668765	-2.310011	0.259012
7	1	0	5.227071	-0.901744	-0.231492
8	1	0	3.645134	0.920018	-0.799908
9	1	0	1.904784	-3.469778	0.700868
10	1	0	4.351908	-3.113544	0.514350
11	7	0	-0.011600	-1.713097	0.091882
12	6	0	-0.730415	-0.593619	0.465406
13	1	0	-0.351388	-0.161975	1.395694
14	6	0	-0.546123	-2.738990	-0.811590
15	1	0	-1.583836	-2.945423	-0.552390
16	1	0	-0.484059	-2.442494	-1.865783
17	1	0	0.033128	-3.652789	-0.677421

18	6	0	-2.192886	-0.447880	0.299656
19	6	0	-2.941347	-0.048264	1.421735
20	6	0	-2.851265	-0.614318	-0.933471
21	6	0	-4.318560	0.140193	1.324547
22	1	0	-2.440407	0.101817	2.373461
23	6	0	-4.226006	-0.415724	-1.027950
24	1	0	-2.287837	-0.873309	-1.822864
25	6	0	-4.964003	-0.045015	0.100268
26	1	0	-4.884889	0.436041	2.201835
27	1	0	-4.721490	-0.542681	-1.985166
28	1	0	-6.035814	0.107998	0.021557
29	6	0	0.947168	0.894501	-0.756537
30	6	0	1.154081	2.217275	-0.229783
31	1	0	0.681925	0.898484	-1.818493
32	6	0	0.584520	3.334870	-0.882320
33	7	0	0.121732	4.256896	-1.434923
34	6	0	1.778775	2.446101	1.018385
35	7	0	2.302091	2.650259	2.045257
36	1	0	-0.167671	0.419809	-0.298819

0662dab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_TS_HC.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.155066	-1.047084	-0.058517
2	6	0	3.267745	-0.021829	-0.385506
3	6	0	1.884308	-0.218023	-0.352351
4	6	0	1.406414	-1.492393	0.013992
5	6	0	2.290647	-2.521293	0.347172
6	6	0	3.665710	-2.300962	0.305863
7	1	0	5.224013	-0.860013	-0.074918
8	1	0	3.641292	0.958599	-0.664231
9	1	0	1.898771	-3.485354	0.656255
10	1	0	4.347912	-3.101550	0.573674
11	7	0	-0.012628	-1.735561	0.027954
12	6	0	-0.763315	-0.676675	0.465530
13	1	0	-0.341968	-0.212935	1.358123
14	6	0	-0.522688	-2.773907	-0.866616
15	1	0	-1.541280	-3.036424	-0.580639
16	1	0	-0.508323	-2.465640	-1.920796
17	1	0	0.107136	-3.658494	-0.767208
18	6	0	-2.205360	-0.494939	0.304703
19	6	0	-2.902071	0.084439	1.386447
20	6	0	-2.922309	-0.776085	-0.878479
21	6	0	-4.267348	0.337193	1.304399
22	1	0	-2.361752	0.328800	2.296328
23	6	0	-4.286142	-0.516408	-0.955951
24	1	0	-2.409252	-1.162603	-1.751004
25	6	0	-4.966140	0.033189	0.134660
26	1	0	-4.784579	0.776412	2.151534
27	1	0	-4.819828	-0.731076	-1.876606
28	1	0	-6.030481	0.235222	0.066559
29	6	0	0.945755	0.901329	-0.766928
30	6	0	1.187373	2.240776	-0.256065
31	1	0	0.777435	0.917784	-1.850345
32	6	0	0.702645	3.354076	-0.979108
33	7	0	0.303218	4.254230	-1.610477
34	6	0	1.688237	2.441006	1.050510
35	7	0	2.105745	2.578369	2.135092
36	1	0	-0.124600	0.503556	-0.367238

0662eab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMacn_TS_HC.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.197368	-0.892303	-0.566351
2	6	0	-3.260540	0.110720	-0.788500
3	6	0	-1.888055	-0.121532	-0.609915

4	6	0	-1.474935	-1.395176	-0.151712
5	6	0	-2.424711	-2.401818	0.081877
6	6	0	-3.774638	-2.152751	-0.129183
7	1	0	-5.250640	-0.697248	-0.739712
8	1	0	-3.581105	1.093840	-1.119495
9	1	0	-2.098142	-3.380623	0.415308
10	1	0	-4.498292	-2.943238	0.042005
11	7	0	-0.100979	-1.613565	0.134735
12	6	0	0.771895	-0.898870	-0.663354
13	1	0	0.592085	-1.067142	-1.726949
14	6	0	0.249001	-2.104229	1.473670
15	1	0	1.302071	-2.378769	1.495010
16	1	0	0.046830	-1.356941	2.249538
17	1	0	-0.343481	-2.993445	1.688790
18	6	0	2.189922	-0.656332	-0.321765
19	6	0	3.165012	-0.925592	-1.298507
20	6	0	2.589546	-0.090690	0.903640
21	6	0	4.511084	-0.672990	-1.042371
22	1	0	2.864199	-1.343544	-2.254627
23	6	0	3.935158	0.168073	1.151747
24	1	0	1.848367	0.165734	1.652848
25	6	0	4.899106	-0.127639	0.183567
26	1	0	5.254901	-0.897397	-1.800231
27	1	0	4.231251	0.607987	2.098713
28	1	0	5.947093	0.074929	0.381354
29	6	0	-0.913316	0.996168	-0.849835
30	6	0	-1.005785	2.179616	-0.037020
31	1	0	-0.737400	1.210319	-1.906837
32	6	0	-0.509496	3.416076	-0.510071
33	7	0	-0.103964	4.436411	-0.914986
34	6	0	-1.456122	2.120298	1.302236
35	7	0	-1.825135	2.066226	2.411532
36	1	0	0.198254	0.375866	-0.663592

0662eab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdce_TS_HC_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.231013	-0.812357	-0.610887
2	6	0	-3.271153	0.164467	-0.855610
3	6	0	-1.908888	-0.085802	-0.635231
4	6	0	-1.532484	-1.345345	-0.117036
5	6	0	-2.502053	-2.324774	0.139123
6	6	0	-3.843107	-2.060306	-0.111322
7	1	0	-5.276727	-0.605246	-0.813824
8	1	0	-3.567479	1.138846	-1.232044
9	1	0	-2.196343	-3.292471	0.522420
10	1	0	-4.586134	-2.828374	0.078035
11	7	0	-0.163781	-1.576114	0.203882
12	6	0	0.727429	-0.952290	-0.648026
13	1	0	0.539355	-1.202862	-1.693822
14	6	0	0.147604	-1.895139	1.602887
15	1	0	1.186719	-2.210773	1.682308
16	1	0	-0.032099	-1.041551	2.267968
17	1	0	-0.491761	-2.718600	1.921663
18	6	0	2.151688	-0.717621	-0.328438
19	6	0	3.116545	-1.097804	-1.278466
20	6	0	2.571100	-0.056312	0.841478
21	6	0	4.469529	-0.859526	-1.047845
22	1	0	2.801483	-1.590310	-2.193678
23	6	0	3.924155	0.187688	1.063287
24	1	0	1.841456	0.286585	1.566736
25	6	0	4.876406	-0.218138	0.124316
26	1	0	5.204279	-1.169741	-1.784015
27	1	0	4.234933	0.702425	1.966829
28	1	0	5.930049	-0.026430	0.301831
29	6	0	-0.900879	1.000444	-0.893386
30	6	0	-0.917025	2.164751	-0.048606
31	1	0	-0.762771	1.231814	-1.952291
32	6	0	-0.401080	3.397431	-0.511392
33	7	0	0.018358	4.414007	-0.910741
34	6	0	-1.290085	2.069068	1.312180

35	7	0	-1.588150	1.967245	2.439404
36	1	0	0.189923	0.340109	-0.748083

0662eab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMtol_TS_HC_f3.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.960963	-1.416603	0.254446
2	6	0	-3.250337	-0.282689	-0.101520
3	6	0	-1.868579	-0.300514	-0.399561
4	6	0	-1.141815	-1.539324	-0.272272
5	6	0	-1.911051	-2.684389	0.059935
6	6	0	-3.272747	-2.628442	0.317051
7	1	0	-5.025711	-1.360003	0.451133
8	1	0	-3.777036	0.659129	-0.210981
9	1	0	-1.426491	-3.648805	0.112771
10	1	0	-3.798613	-3.547086	0.560348
11	7	0	0.241834	-1.677654	-0.322750
12	6	0	1.149045	-0.846990	-1.114901
13	1	0	1.455038	-1.388677	-2.022597
14	6	0	0.840624	-2.950015	0.074430
15	1	0	1.917010	-2.805721	0.169681
16	1	0	0.458448	-3.274283	1.045117
17	1	0	0.665062	-3.749329	-0.660476
18	6	0	2.384261	-0.393057	-0.353532
19	6	0	3.643736	-0.441929	-0.960527
20	6	0	2.274813	0.130447	0.941587
21	6	0	4.775192	0.030005	-0.291413
22	1	0	3.740549	-0.851101	-1.963371
23	6	0	3.403877	0.597447	1.613306
24	1	0	1.302140	0.162806	1.424010
25	6	0	4.657467	0.550514	0.997580
26	1	0	5.746468	-0.015406	-0.775197
27	1	0	3.305405	1.000760	2.616873
28	1	0	5.536046	0.915227	1.521317
29	6	0	-1.328215	0.975568	-0.867650
30	6	0	-1.492110	2.188355	-0.260545
31	1	0	-0.822847	1.013400	-1.828046
32	6	0	-1.044867	3.387148	-0.909082
33	7	0	-0.677990	4.356960	-1.437095
34	6	0	-2.067935	2.356458	1.042391
35	7	0	-2.512408	2.529575	2.103544
36	1	0	0.622111	0.034994	-1.464813

0662eab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMw_TS_HC_f4.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.195099	-0.898371	-0.562877
2	6	0	-3.259941	0.106360	-0.784197
3	6	0	-1.886759	-0.124397	-0.608401
4	6	0	-1.470892	-1.398642	-0.153640
5	6	0	-2.419279	-2.406925	0.079248
6	6	0	-3.769843	-2.159185	-0.129107
7	1	0	-5.248865	-0.704486	-0.734518
8	1	0	-3.582297	1.089603	-1.113071
9	1	0	-2.091205	-3.386148	0.409851
10	1	0	-4.492054	-2.951142	0.041345
11	7	0	-0.096650	-1.615815	0.130324
12	6	0	0.774428	-0.894329	-0.664132
13	1	0	0.595598	-1.058277	-1.728582
14	6	0	0.256320	-2.115567	1.465106
15	1	0	1.310170	-2.387235	1.482992
16	1	0	0.053262	-1.374531	2.246682
17	1	0	-0.333052	-3.008183	1.674445
18	6	0	2.192352	-0.651672	-0.321058
19	6	0	3.168079	-0.915492	-1.298553
20	6	0	2.590652	-0.091079	0.907052

21	6	0	4.513791	-0.662478	-1.040593
22	1	0	2.868181	-1.329512	-2.256656
23	6	0	3.935854	0.168088	1.157046
24	1	0	1.848672	0.160844	1.657009
25	6	0	4.900607	-0.122183	0.187969
26	1	0	5.258230	-0.882690	-1.799068
27	1	0	4.231036	0.603885	2.106202
28	1	0	5.948284	0.080581	0.387210
29	6	0	-0.914589	0.995344	-0.847586
30	6	0	-1.011655	2.179965	-0.037386
31	1	0	-0.734384	1.207461	-1.904199
32	6	0	-0.515639	3.416422	-0.510656
33	7	0	-0.110329	4.437139	-0.914916
34	6	0	-1.468351	2.123720	1.299842
35	7	0	-1.843193	2.073818	2.407390
36	1	0	0.199391	0.376352	-0.657700

0662eab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_vacuol_TS_HC_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.328224	-0.492157	-0.645737
2	6	0	-3.294966	0.397968	-0.926184
3	6	0	-1.961562	0.061692	-0.664396
4	6	0	-1.689011	-1.190303	-0.076359
5	6	0	-2.727021	-2.083242	0.213757
6	6	0	-4.042289	-1.735006	-0.073517
7	1	0	-5.353456	-0.219281	-0.874771
8	1	0	-3.514489	1.372203	-1.353101
9	1	0	-2.495548	-3.047945	0.653833
10	1	0	-4.843844	-2.433730	0.144705
11	7	0	-0.335912	-1.501756	0.266982
12	6	0	0.595150	-1.092132	-0.660733
13	1	0	0.371027	-1.446908	-1.668370
14	6	0	-0.039652	-1.697643	1.691429
15	1	0	0.969406	-2.094782	1.799532
16	1	0	-0.143547	-0.768012	2.266258
17	1	0	-0.747570	-2.426843	2.089102
18	6	0	2.018992	-0.874141	-0.369775
19	6	0	2.975169	-1.375481	-1.273369
20	6	0	2.457038	-0.096643	0.721871
21	6	0	4.331774	-1.140213	-1.073628
22	1	0	2.646435	-1.960078	-2.128255
23	6	0	3.815924	0.141416	0.910827
24	1	0	1.738012	0.341751	1.405267
25	6	0	4.756005	-0.382829	0.020981
26	1	0	5.057896	-1.543418	-1.772744
27	1	0	4.139910	0.748565	1.750198
28	1	0	5.813941	-0.192536	0.173387
29	6	0	-0.854363	1.046215	-0.950137
30	6	0	-0.643429	2.118992	-0.007068
31	1	0	-0.837211	1.383611	-1.989577
32	6	0	-0.071330	3.343195	-0.430197
33	7	0	0.389675	4.347824	-0.809500
34	6	0	-0.798641	1.873653	1.375343
35	7	0	-0.901054	1.590609	2.507261
36	1	0	0.132687	0.290621	-0.947320

0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.509045	2.395615	0.542559
2	6	0	-3.518121	1.144053	-0.071856
3	6	0	-2.340850	0.498758	-0.472952
4	6	0	-1.102499	1.151446	-0.229617
5	6	0	-1.111674	2.414989	0.375124
6	6	0	-2.295730	3.038391	0.767196

7	1	0	-4.444248	2.858350	0.842636
8	1	0	-4.466865	0.642239	-0.242106
9	1	0	-0.156391	2.905065	0.534655
10	1	0	-2.264478	4.013624	1.243341
11	7	0	0.207917	0.653349	-0.596887
12	6	0	0.866734	-0.326628	0.211306
13	1	0	0.477891	-0.227459	1.229634
14	6	0	0.587379	0.776325	-2.004116
15	1	0	0.310609	1.771532	-2.361735
16	1	0	1.670128	0.665398	-2.097505
17	1	0	0.112675	0.030934	-2.657767
18	6	0	2.383928	-0.190921	0.229324
19	6	0	3.233044	-1.274092	-0.012046
20	6	0	2.942310	1.052741	0.556438
21	6	0	4.618719	-1.116249	0.070841
22	1	0	2.805080	-2.236238	-0.268033
23	6	0	4.324000	1.209138	0.639820
24	1	0	2.286743	1.898607	0.739851
25	6	0	5.168072	0.122745	0.396319
26	1	0	5.266999	-1.965996	-0.122079
27	1	0	4.742420	2.178493	0.894681
28	1	0	6.245445	0.243690	0.460257
29	6	0	-2.473100	-0.878117	-1.117766
30	6	0	-1.994378	-2.001442	-0.175422
31	1	0	-3.516980	-1.056978	-1.388249
32	6	0	-2.879888	-2.689376	0.688556
33	7	0	-3.646007	-3.243202	1.371439
34	6	0	-0.666055	-2.056646	-0.109077
35	7	0	0.498865	-1.755127	-0.270657
36	1	0	-1.891531	-0.930764	-2.042633

0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMacn.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.813802	2.743737	0.472471
2	6	0	-2.880630	1.376633	0.201776
3	6	0	-1.751700	0.642722	-0.179469
4	6	0	-0.544423	1.356095	-0.268428
5	6	0	-0.452954	2.722286	0.005222
6	6	0	-1.598415	3.422167	0.379470
7	1	0	-3.713204	3.278104	0.762657
8	1	0	-3.820189	0.843632	0.301166
9	1	0	0.503240	3.227127	-0.087328
10	1	0	-1.536964	4.484023	0.593031
11	7	0	0.679536	0.669043	-0.673551
12	6	0	1.622419	0.510984	0.218774
13	1	0	1.355005	0.898891	1.197423
14	6	0	0.788837	0.291915	-2.097985
15	1	0	1.721103	0.684920	-2.506622
16	1	0	0.753247	-0.793039	-2.210131
17	1	0	-0.049575	0.737842	-2.627106
18	6	0	2.941670	-0.066098	0.126348
19	6	0	3.744968	0.130729	1.276662
20	6	0	3.476852	-0.799691	-0.959832
21	6	0	5.042892	-0.357956	1.330469
22	1	0	3.339671	0.677285	2.122271
23	6	0	4.772361	-1.294880	-0.890230
24	1	0	2.891267	-1.009550	-1.842025
25	6	0	5.558767	-1.070871	0.245133
26	1	0	5.647988	-0.190986	2.214739
27	1	0	5.171629	-1.862017	-1.723950
28	1	0	6.570953	-1.460374	0.285197
29	6	0	-1.831343	-0.858059	-0.473420
30	6	0	-3.020923	-1.601221	0.104921
31	1	0	-1.840097	-0.993187	-1.562774
32	6	0	-4.121149	-1.921585	-0.693767
33	7	0	-5.038148	-2.193268	-1.382865
34	6	0	-3.026074	-1.977064	1.451419
35	7	0	-3.004041	-2.289598	2.587233
36	1	0	-0.899623	-1.324967	-0.129480

0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMdce.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.834135	2.729148	0.496030
2	6	0	-2.893673	1.366330	0.204539
3	6	0	-1.760392	0.644484	-0.187300
4	6	0	-0.557310	1.365537	-0.262633
5	6	0	-0.472445	2.727914	0.032636
6	6	0	-1.622109	3.415679	0.415410
7	1	0	-3.736618	3.254137	0.793577
8	1	0	-3.829508	0.825479	0.296266
9	1	0	0.481275	3.239415	-0.049799
10	1	0	-1.566844	4.474354	0.645979
11	7	0	0.670994	0.689897	-0.675787
12	6	0	1.609542	0.515390	0.217895
13	1	0	1.335562	0.883439	1.202472
14	6	0	0.785851	0.338174	-2.106064
15	1	0	1.717157	0.742493	-2.506185
16	1	0	0.755467	-0.744927	-2.237127
17	1	0	-0.054192	0.788208	-2.629153
18	6	0	2.929990	-0.058764	0.121848
19	6	0	3.725907	0.114018	1.281088
20	6	0	3.472380	-0.769891	-0.975663
21	6	0	5.023219	-0.376339	1.333483
22	1	0	3.315087	0.642713	2.135462
23	6	0	4.767228	-1.266921	-0.907760
24	1	0	2.892570	-0.961492	-1.865850
25	6	0	5.546061	-1.066975	0.237215
26	1	0	5.622309	-0.228497	2.225215
27	1	0	5.171787	-1.817297	-1.750150
28	1	0	6.557628	-1.458204	0.276171
29	6	0	-1.834270	-0.851559	-0.505762
30	6	0	-2.998140	-1.615426	0.095411
31	1	0	-1.875953	-0.965749	-1.596921
32	6	0	-4.112348	-1.943382	-0.681225
33	7	0	-5.039030	-2.217869	-1.355601
34	6	0	-2.957138	-2.002949	1.438419
35	7	0	-2.890196	-2.321513	2.570518
36	1	0	-0.887404	-1.314491	-0.199269

0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMtol.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.619310	2.048398	0.781179
2	6	0	-3.388116	0.931844	-0.016113
3	6	0	-2.096344	0.573522	-0.435267
4	6	0	-1.049242	1.397795	0.001524
5	6	0	-1.259219	2.521004	0.807651
6	6	0	-2.552582	2.848265	1.201557
7	1	0	-4.633163	2.293480	1.082010
8	1	0	-4.218877	0.300228	-0.316224
9	1	0	-0.412429	3.123292	1.122598
10	1	0	-2.724214	3.713756	1.832916
11	7	0	0.328683	1.138315	-0.418294
12	6	0	1.096928	0.389678	0.328895
13	1	0	0.578891	-0.114376	1.141814
14	6	0	0.734749	1.782105	-1.681028
15	1	0	1.026667	2.820022	-1.499841
16	1	0	1.559084	1.232981	-2.133594
17	1	0	-0.127570	1.772942	-2.346860
18	6	0	2.508660	0.099544	0.182657
19	6	0	2.935886	-1.135451	0.722609
20	6	0	3.460304	0.976269	-0.385808
21	6	0	4.275946	-1.499977	0.646792
22	1	0	2.193936	-1.803409	1.152984
23	6	0	4.799765	0.610769	-0.427365

24	1	0	3.170158	1.955823	-0.744920
25	6	0	5.207240	-0.630171	0.075373
26	1	0	4.594770	-2.458729	1.041923
27	1	0	5.530458	1.294563	-0.846548
28	1	0	6.254912	-0.911261	0.030421
29	6	0	-1.889103	-0.695952	-1.251633
30	6	0	-1.994682	-1.959932	-0.404603
31	1	0	-2.653410	-0.734000	-2.033948
32	6	0	-3.200380	-2.670056	-0.352799
33	7	0	-4.224649	-3.247365	-0.346055
34	6	0	-0.948003	-2.259586	0.460274
35	7	0	-0.011507	-2.433192	1.158777
36	1	0	-0.921879	-0.658019	-1.767090

0663bab_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.808754	2.747659	0.464562
2	6	0	-2.877602	1.379465	0.199546
3	6	0	-1.749764	0.642185	-0.178319
4	6	0	-0.541288	1.353311	-0.270547
5	6	0	-0.447963	2.720474	-0.002655
6	6	0	-1.592325	3.423729	0.368790
7	1	0	-3.707371	3.284666	0.752319
8	1	0	-3.818248	0.848712	0.300683
9	1	0	0.508984	3.223376	-0.097577
10	1	0	-1.529157	4.486381	0.577799
11	7	0	0.681499	0.663079	-0.673211
12	6	0	1.625731	0.510111	0.218613
13	1	0	1.360070	0.903703	1.195441
14	6	0	0.789152	0.278367	-2.095811
15	1	0	1.721205	0.668828	-2.507234
16	1	0	0.753050	-0.807123	-2.202170
17	1	0	-0.049378	0.722112	-2.626558
18	6	0	2.944737	-0.067660	0.127419
19	6	0	3.749709	0.135496	1.275470
20	6	0	3.478285	-0.807212	-0.955514
21	6	0	5.047710	-0.352929	1.330051
22	1	0	3.345701	0.686846	2.118549
23	6	0	4.773902	-1.302039	-0.885093
24	1	0	2.891413	-1.021831	-1.835685
25	6	0	5.561986	-1.071800	0.247871
26	1	0	5.654137	-0.180986	2.212456
27	1	0	5.171963	-1.873636	-1.716334
28	1	0	6.574263	-1.461005	0.288547
29	6	0	-1.830994	-0.859813	-0.465345
30	6	0	-3.026612	-1.597449	0.108145
31	1	0	-1.832281	-1.000844	-1.553928
32	6	0	-4.122756	-1.918256	-0.695773
33	7	0	-5.036886	-2.191112	-1.388342
34	6	0	-3.043580	-1.967636	1.456009
35	7	0	-3.033011	-2.275949	2.593210
36	1	0	-0.903001	-1.327355	-0.112417

0663bac_Ph_NMeBn_CHC_CN_CN_ZWion_B3lyp631pd.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.507188	-2.391821	-0.591589
2	6	0	-3.528083	-1.146343	0.035113
3	6	0	-2.357191	-0.501165	0.454143
4	6	0	-1.118025	-1.149189	0.215187
5	6	0	-1.111302	-2.406722	-0.400144
6	6	0	-2.289758	-3.029354	-0.810198
7	1	0	-4.437344	-2.854744	-0.906627
8	1	0	-4.480004	-0.649064	0.199920
9	1	0	-0.153236	-2.892396	-0.557628

10	1	0	-2.250975	-3.999403	-1.296100
11	7	0	0.180476	-0.631747	0.598332
12	6	0	0.858622	0.286821	-0.222458
13	1	0	0.484815	0.117134	-1.267565
14	6	0	0.566132	-0.784195	2.002134
15	1	0	0.313755	-1.794211	2.335352
16	1	0	1.644177	-0.644227	2.099443
17	1	0	0.068017	-0.064775	2.664627
18	6	0	2.376186	0.170854	-0.221460
19	6	0	3.219619	1.282011	-0.131838
20	6	0	2.943954	-1.098632	-0.408450
21	6	0	4.604286	1.126218	-0.225442
22	1	0	2.787819	2.263310	0.020663
23	6	0	4.325859	-1.252784	-0.499134
24	1	0	2.296236	-1.967224	-0.478641
25	6	0	5.162175	-0.138266	-0.408163
26	1	0	5.246210	1.999045	-0.150789
27	1	0	4.748817	-2.243053	-0.641084
28	1	0	6.239430	-0.256466	-0.478252
29	6	0	-2.489065	0.866190	1.118421
30	6	0	-1.980316	2.005606	0.218409
31	1	0	-3.537413	1.046281	1.370578
32	6	0	-2.841101	2.689267	-0.673504
33	7	0	-3.587815	3.237861	-1.382384
34	6	0	-0.648546	2.103196	0.200950
35	7	0	0.527538	1.859387	0.372098
36	1	0	-1.929254	0.891141	2.057922

0701aaa_Ph_NMeBn_CHC_CN_Me_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.329604	-0.637985	0.035337
2	6	0	3.394212	0.388442	-0.057547
3	6	0	2.015910	0.125437	-0.160085
4	6	0	1.569242	-1.229757	-0.150854
5	6	0	2.529043	-2.252600	-0.068170
6	6	0	3.889429	-1.961788	0.022165
7	1	0	5.388137	-0.406681	0.094915
8	1	0	3.737720	1.415165	-0.113599
9	1	0	2.212832	-3.288378	-0.055834
10	1	0	4.603997	-2.776842	0.090290
11	7	0	0.186844	-1.516877	-0.258598
12	6	0	-0.673283	-1.036879	0.835981
13	1	0	-0.224724	-0.130696	1.251511
14	1	0	-0.687141	-1.774799	1.655661
15	6	0	-0.171991	-2.870016	-0.681225
16	1	0	-1.232259	-2.884503	-0.941363
17	1	0	0.401907	-3.151154	-1.566515
18	1	0	-0.007715	-3.625291	0.103841
19	6	0	-2.104947	-0.730315	0.425722
20	6	0	-3.114246	-0.771956	1.397557
21	6	0	-2.446930	-0.357958	-0.880131
22	6	0	-4.429831	-0.434327	1.077941
23	1	0	-2.866653	-1.070666	2.413448
24	6	0	-3.764806	-0.027003	-1.204952
25	1	0	-1.678701	-0.345126	-1.646778
26	6	0	-4.760284	-0.059818	-0.226966
27	1	0	-5.197519	-0.471253	1.845512
28	1	0	-4.012155	0.254953	-2.224439
29	1	0	-5.784725	0.197316	-0.479472
30	6	0	1.055234	1.199952	-0.415621
31	6	0	1.059725	2.470654	0.062438
32	1	0	0.237314	0.923603	-1.076675
33	6	0	0.040083	3.353226	-0.425801
34	7	0	-0.774989	4.096899	-0.802493
35	6	0	2.001460	3.065952	1.085605
36	1	0	2.496900	2.281347	1.659479
37	1	0	2.772687	3.683666	0.611290
38	1	0	1.451381	3.709630	1.777995

0702dab_Ph_NMeBn_CHC_CN_Me_ZWion_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.200544	-0.968003	0.145098
2	6	0	3.321943	0.091506	-0.088378
3	6	0	1.939030	-0.104125	-0.149472
4	6	0	1.454660	-1.417120	0.011911
5	6	0	2.326658	-2.484756	0.243435
6	6	0	3.701277	-2.261043	0.308164
7	1	0	5.268505	-0.782049	0.204204
8	1	0	3.699857	1.100216	-0.232817
9	1	0	1.925832	-3.484349	0.379004
10	1	0	4.374236	-3.092068	0.494018
11	7	0	0.040001	-1.658107	-0.099667
12	6	0	-0.751966	-0.727911	0.506623
13	1	0	-0.375500	-0.428399	1.482821
14	6	0	-0.406255	-2.531823	-1.188177
15	1	0	-1.427637	-2.860628	-0.998678
16	1	0	-0.355470	-2.037068	-2.165612
17	1	0	0.242095	-3.407641	-1.215566
18	6	0	-2.179165	-0.510617	0.299320
19	6	0	-2.938691	-0.126143	1.427160
20	6	0	-2.832740	-0.586219	-0.951223
21	6	0	-4.299968	0.137783	1.317898
22	1	0	-2.449873	-0.046990	2.393834
23	6	0	-4.193797	-0.316219	-1.053731
24	1	0	-2.274983	-0.823503	-1.848545
25	6	0	-4.935573	0.039546	0.077114
26	1	0	-4.865290	0.421233	2.200178
27	1	0	-4.677041	-0.374558	-2.024041
28	1	0	-5.997221	0.247788	-0.010842
29	6	0	1.009152	1.055578	-0.489697
30	6	0	1.306712	2.376585	0.045615
31	1	0	0.840869	1.093070	-1.573510
32	6	0	0.945164	3.492074	-0.712395
33	7	0	0.676991	4.443475	-1.355659
34	1	0	-0.044352	0.670520	-0.092961
35	6	0	1.647570	2.577881	1.502685
36	1	0	2.357098	1.819462	1.851189
37	1	0	2.091041	3.562476	1.678563
38	1	0	0.761558	2.503073	2.154353

0703aab_Ph_NMeBn_CHC_CN_Me_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.939823	2.715835	0.463468
2	6	0	-3.041524	1.352880	0.184196
3	6	0	-1.927187	0.588368	-0.181102
4	6	0	-0.695111	1.259683	-0.248620
5	6	0	-0.574063	2.624293	0.028898
6	6	0	-1.703013	3.358284	0.388232
7	1	0	-3.826085	3.275452	0.747732
8	1	0	-3.994475	0.839349	0.266791
9	1	0	0.398372	3.100881	-0.048258
10	1	0	-1.612623	4.417324	0.607029
11	7	0	0.515486	0.544093	-0.628020
12	6	0	1.473600	0.426990	0.272269
13	1	0	1.158139	0.717827	1.269630
14	6	0	0.647436	0.182330	-2.050715
15	1	0	1.210184	0.954936	-2.582473
16	1	0	1.144284	-0.782502	-2.147492
17	1	0	-0.349570	0.120323	-2.479702
18	6	0	2.825283	-0.055872	0.164100
19	6	0	3.463689	-0.321910	1.403457
20	6	0	3.566456	-0.256294	-1.028026
21	6	0	4.765881	-0.798109	1.450504
22	1	0	2.916663	-0.157553	2.326636

23	6	0	4.873868	-0.721894	-0.967825
24	1	0	3.146540	-0.022288	-1.995249
25	6	0	5.476098	-1.003351	0.263262
26	1	0	5.230665	-1.004265	2.408873
27	1	0	5.430729	-0.861918	-1.888425
28	1	0	6.496717	-1.370732	0.296376
29	6	0	-2.058074	-0.903707	-0.498468
30	6	0	-3.063106	-1.660530	0.322845
31	1	0	-2.318460	-0.997115	-1.561895
32	6	0	-4.072698	-2.361125	-0.300089
33	7	0	-4.954244	-2.955343	-0.834600
34	1	0	-1.042010	-1.333906	-0.407205
35	6	0	-2.804702	-1.827116	1.799915
36	1	0	-2.684261	-0.859464	2.313535
37	1	0	-3.628182	-2.352044	2.295144
38	1	0	-1.883375	-2.398072	2.019469

0711aaa_Ph_NMeBn_CHC_CN_Me_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.644739	-0.154952	0.265578
2	6	0	3.728527	0.889054	0.133687
3	6	0	2.375532	0.651031	-0.113923
4	6	0	1.899894	-0.678235	-0.203178
5	6	0	2.832606	-1.729183	-0.069596
6	6	0	4.182071	-1.466581	0.157961
7	1	0	5.694100	0.052804	0.448567
8	1	0	4.066885	1.919787	0.208871
9	1	0	2.502507	-2.758797	-0.130458
10	1	0	4.871444	-2.300390	0.256984
11	7	0	0.539609	-0.959725	-0.392924
12	6	0	-0.439654	0.117613	-0.595828
13	1	0	-0.466141	0.409373	-1.658332
14	6	0	0.218917	-2.235205	-1.042708
15	1	0	-0.811414	-2.217344	-1.392919
16	1	0	0.874414	-2.418908	-1.903460
17	1	0	0.315074	-3.077224	-0.349184
18	6	0	-1.851122	-0.326592	-0.218115
19	6	0	-2.934226	0.078058	-1.008969
20	6	0	-2.102661	-1.116905	0.913386
21	6	0	-4.240891	-0.279384	-0.669424
22	1	0	-2.754729	0.674806	-1.899027
23	6	0	-3.406784	-1.478158	1.252063
24	1	0	-1.270452	-1.462335	1.517939
25	6	0	-4.481174	-1.057290	0.463953
26	1	0	-5.067107	0.043273	-1.295909
27	1	0	-3.583342	-2.092447	2.130111
28	1	0	-5.495677	-1.341614	0.726841
29	6	0	1.418109	1.797937	-0.316556
30	6	0	0.003316	1.413338	0.185221
31	1	0	1.767785	2.689573	0.212504
32	1	0	1.357342	2.064558	-1.379227
33	6	0	-0.917391	2.505853	-0.174219
34	7	0	-1.613836	3.394061	-0.448832
35	6	0	-0.008348	1.255061	1.722803
36	1	0	0.347952	2.176948	2.189882
37	1	0	-1.011495	1.044409	2.095364
38	1	0	0.653664	0.440416	2.020929

0801aaa_Ph_NMeBn_CHC_Me_Me_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.273483	-0.761923	0.048908
2	6	0	3.412569	0.319885	-0.135815
3	6	0	2.020428	0.159794	-0.232950
4	6	0	1.483065	-1.157678	-0.139764

5	6	0	2.362487	-2.239192	0.034347
6	6	0	3.741756	-2.047323	0.126364
7	1	0	5.345706	-0.600948	0.107085
8	1	0	3.828559	1.314499	-0.258087
9	1	0	1.968816	-3.245619	0.112770
10	1	0	4.393006	-2.906030	0.262727
11	7	0	0.079309	-1.358468	-0.262420
12	6	0	-0.742932	-0.769909	0.806888
13	1	0	-0.266163	0.162119	1.121528
14	1	0	-0.754574	-1.431201	1.690632
15	6	0	-0.357899	-2.709770	-0.603643
16	1	0	-1.413790	-2.677401	-0.880868
17	1	0	0.209898	-3.082514	-1.459016
18	1	0	-0.252302	-3.426240	0.228103
19	6	0	-2.175481	-0.467165	0.399723
20	6	0	-3.193239	-0.528848	1.360859
21	6	0	-2.507675	-0.070776	-0.902531
22	6	0	-4.507872	-0.189190	1.035863
23	1	0	-2.953572	-0.845619	2.373182
24	6	0	-3.822952	0.261818	-1.233072
25	1	0	-1.730458	-0.041157	-1.659380
26	6	0	-4.827770	0.207935	-0.264375
27	1	0	-5.282317	-0.242963	1.795729
28	1	0	-4.062697	0.562399	-2.249204
29	1	0	-5.850757	0.466532	-0.521595
30	6	0	1.142565	1.303185	-0.547717
31	6	0	1.181070	2.562257	-0.065458
32	1	0	0.359447	1.073133	-1.269020
33	6	0	2.108770	3.046879	1.021068
34	1	0	2.618189	2.231083	1.536620
35	1	0	2.874480	3.723113	0.617812
36	1	0	1.546147	3.627550	1.762547
37	6	0	0.228536	3.607570	-0.592680
38	1	0	-0.432462	3.208415	-1.366563
39	1	0	-0.392289	4.017484	0.214667
40	1	0	0.778519	4.457352	-1.018813

0803aab_Ph_NMeBn_CHC_Me_Me_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.249020	2.503268	-0.415119
2	6	0	3.349761	1.154797	-0.068888
3	6	0	2.214685	0.407772	0.266368
4	6	0	0.970400	1.055501	0.263289
5	6	0	0.861355	2.405959	-0.081061
6	6	0	2.002061	3.132678	-0.422322
7	1	0	4.141492	3.060168	-0.685505
8	1	0	4.314666	0.656359	-0.077084
9	1	0	-0.118212	2.875159	-0.075301
10	1	0	1.916039	4.181563	-0.689729
11	7	0	-0.214231	0.307831	0.630190
12	6	0	-1.224375	0.289058	-0.295455
13	1	0	-0.854527	0.454100	-1.301526
14	6	0	-0.454926	0.196067	2.075400
15	1	0	-1.031519	1.050674	2.452137
16	1	0	-0.986051	-0.729540	2.298120
17	1	0	0.506880	0.176013	2.586406
18	6	0	-2.608571	-0.013954	-0.187240
19	6	0	-3.320475	-0.117929	-1.427538
20	6	0	-3.385371	-0.209971	0.998140
21	6	0	-4.674740	-0.397976	-1.478222
22	1	0	-2.770429	0.026465	-2.353892
23	6	0	-4.744163	-0.492545	0.928278
24	1	0	-2.935413	-0.123148	1.976582
25	6	0	-5.409958	-0.594719	-0.298793
26	1	0	-5.167709	-0.467746	-2.444301
27	1	0	-5.296548	-0.631611	1.854084
28	1	0	-6.471489	-0.816858	-0.336942
29	6	0	2.278077	-1.057297	0.665704
30	6	0	3.075741	-1.958348	-0.188944
31	1	0	2.616540	-1.144530	1.709471

32	1	0	1.186780	-1.346840	0.704480
33	6	0	2.890753	-1.939272	-1.669855
34	1	0	2.660231	-0.936148	-2.045968
35	1	0	3.782361	-2.309389	-2.194284
36	1	0	2.058915	-2.594194	-2.003039
37	6	0	3.672129	-3.185138	0.416425
38	1	0	2.978834	-4.052213	0.413265
39	1	0	4.557465	-3.521474	-0.141596
40	1	0	3.962899	-3.029332	1.462299

0811aaa_Ph_NMeBn_CHC_Me_Me_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.565611	-0.261728	0.320931
2	6	0	3.708671	0.824209	0.125090
3	6	0	2.350927	0.652247	-0.145179
4	6	0	1.807592	-0.654532	-0.194846
5	6	0	2.678333	-1.748721	0.001529
6	6	0	4.035608	-1.549952	0.252408
7	1	0	5.620547	-0.102953	0.521851
8	1	0	4.101948	1.837731	0.167392
9	1	0	2.292461	-2.760794	-0.026976
10	1	0	4.676600	-2.414869	0.400828
11	7	0	0.444826	-0.863423	-0.420973
12	6	0	-0.487303	0.262274	-0.631353
13	1	0	-0.524727	0.504445	-1.707245
14	6	0	0.064074	-2.138212	-1.031246
15	1	0	-0.936136	-2.055460	-1.454319
16	1	0	0.756597	-2.415939	-1.836304
17	1	0	0.044050	-2.956286	-0.301392
18	6	0	-1.906368	-0.134879	-0.225397
19	6	0	-2.991374	0.239320	-1.029711
20	6	0	-2.166752	-0.864865	0.944333
21	6	0	-4.301659	-0.082550	-0.667708
22	1	0	-2.808917	0.784327	-1.952201
23	6	0	-3.473607	-1.191898	1.307479
24	1	0	-1.336250	-1.190068	1.562302
25	6	0	-4.547692	-0.798241	0.504887
26	1	0	-5.126474	0.218160	-1.307302
27	1	0	-3.653064	-1.758953	2.216520
28	1	0	-5.564504	-1.055802	0.786314
29	6	0	1.445088	1.826372	-0.414512
30	6	0	0.004989	1.573008	0.075634
31	1	0	1.843481	2.728706	0.063720
32	1	0	1.417765	2.037836	-1.493648
33	6	0	-0.010368	1.469705	1.612565
34	1	0	0.405401	2.386780	2.044148
35	1	0	-1.027302	1.353408	1.995397
36	1	0	0.587501	0.629648	1.975611
37	6	0	-0.876239	2.757378	-0.357258
38	1	0	-0.895664	2.865721	-1.447526
39	1	0	-1.906658	2.647519	-0.008774
40	1	0	-0.477629	3.687185	0.062541

0901aaa_Ph_NMeBn_CHC_COOMe_COOMe_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.136150	2.913320	-0.489838
2	6	0	-2.651906	1.610165	-0.499531
3	6	0	-1.273229	1.337436	-0.434346
4	6	0	-0.353695	2.420901	-0.325588
5	6	0	-0.860444	3.732275	-0.334234
6	6	0	-2.230226	3.973832	-0.417535
7	1	0	-4.202441	3.100222	-0.562753
8	1	0	-3.343839	0.783815	-0.625569
9	1	0	-0.183373	4.573550	-0.252828

10	1	0	-2.589370	4.998776	-0.415344
11	7	0	1.031492	2.157599	-0.236005
12	6	0	1.487315	1.377758	0.927363
13	1	0	0.663778	0.739485	1.258511
14	1	0	1.702897	2.056083	1.769683
15	6	0	1.936092	3.265395	-0.540801
16	1	0	2.946633	2.868364	-0.655378
17	1	0	1.646138	3.739768	-1.480413
18	1	0	1.961513	4.029805	0.251759
19	6	0	2.710179	0.511335	0.669165
20	6	0	3.499692	0.112807	1.756900
21	6	0	3.052490	0.056632	-0.609898
22	6	0	4.594307	-0.732773	1.574618
23	1	0	3.253542	0.467114	2.755134
24	6	0	4.153408	-0.783432	-0.796616
25	1	0	2.462179	0.376348	-1.462592
26	6	0	4.925598	-1.184901	0.294588
27	1	0	5.192632	-1.032047	2.430348
28	1	0	4.407423	-1.121399	-1.797286
29	1	0	5.781204	-1.837757	0.149475
30	6	0	-0.771243	-0.023617	-0.612999
31	6	0	-1.327638	-1.180302	-0.185411
32	1	0	0.155557	-0.105934	-1.173815
33	6	0	-0.745942	-2.506726	-0.503220
34	8	0	-1.101263	-3.542407	0.038153
35	8	0	0.225871	-2.452137	-1.433460
36	6	0	-2.491104	-1.231327	0.766253
37	8	0	-2.460507	-0.816271	1.907867
38	8	0	-3.570536	-1.797266	0.201314
39	6	0	0.881454	-3.700973	-1.728556
40	1	0	1.636116	-3.463783	-2.476611
41	1	0	1.348954	-4.109738	-0.830292
42	1	0	0.164743	-4.423679	-2.124036
43	6	0	-4.723197	-1.950416	1.058842
44	1	0	-4.476588	-2.582558	1.914226
45	1	0	-5.066464	-0.976423	1.412887
46	1	0	-5.484773	-2.422889	0.440999

0901aab_Ph_NMeBn_CHC_COOMe_COOMe_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.032647	-3.016762	-0.530146
2	6	0	2.593063	-1.699562	-0.597633
3	6	0	1.224204	-1.376758	-0.540603
4	6	0	0.269910	-2.423342	-0.379089
5	6	0	0.732032	-3.749895	-0.329161
6	6	0	2.092311	-4.041860	-0.406388
7	1	0	4.091710	-3.242638	-0.598124
8	1	0	3.314105	-0.905709	-0.762027
9	1	0	0.027068	-4.562819	-0.206846
10	1	0	2.416740	-5.077206	-0.358616
11	7	0	-1.106219	-2.109596	-0.294499
12	6	0	-1.523839	-1.286956	0.854525
13	1	0	-0.687349	-0.641932	1.136643
14	1	0	-1.717691	-1.933569	1.726714
15	6	0	-2.046037	-3.199257	-0.556514
16	1	0	-3.044066	-2.775755	-0.684269
17	1	0	-1.772790	-3.716637	-1.478227
18	1	0	-2.093325	-3.932934	0.263719
19	6	0	-2.749202	-0.423202	0.601718
20	6	0	-3.531602	-0.019865	1.692609
21	6	0	-3.099110	0.026655	-0.677198
22	6	0	-4.626836	0.825974	1.513791
23	1	0	-3.279643	-0.370665	2.690610
24	6	0	-4.200278	0.866645	-0.860321
25	1	0	-2.514096	-0.296339	-1.532259
26	6	0	-4.965540	1.273070	0.234143
27	1	0	-5.219778	1.128901	2.371989
28	1	0	-4.459453	1.201940	-1.860530
29	1	0	-5.821406	1.926160	0.091570
30	6	0	0.764646	-0.011676	-0.780887

31	6	0	1.356873	1.156700	-0.440736
32	1	0	-0.168112	0.077709	-1.333458
33	6	0	0.729515	2.421419	-0.909651
34	8	0	-0.208950	2.488469	-1.685418
35	8	0	1.302733	3.501714	-0.344466
36	6	0	2.605223	1.252310	0.386062
37	8	0	3.659719	1.714816	-0.005972
38	8	0	2.416990	0.756889	1.620972
39	6	0	0.748136	4.777526	-0.720247
40	1	0	1.332235	5.520261	-0.179345
41	1	0	0.838893	4.930231	-1.797705
42	1	0	-0.304170	4.835307	-0.434213
43	6	0	3.575934	0.757715	2.482477
44	1	0	4.361745	0.127253	2.060659
45	1	0	3.954697	1.773442	2.610692
46	1	0	3.231998	0.353789	3.433085

0902dab_Ph_NMeBn_CHC_COOMe_COOMe_ZWion_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.015379	3.819213	-0.488120
2	6	0	-1.914011	2.444373	-0.709760
3	6	0	-0.705344	1.765429	-0.528397
4	6	0	0.423007	2.516296	-0.139960
5	6	0	0.326057	3.890343	0.087725
6	6	0	-0.892805	4.544859	-0.089030
7	1	0	-2.971763	4.316492	-0.616896
8	1	0	-2.786218	1.875622	-1.018601
9	1	0	1.203921	4.440494	0.411358
10	1	0	-0.963118	5.612309	0.093955
11	7	0	1.690229	1.849266	-0.013749
12	6	0	1.567601	0.549208	0.438288
13	1	0	0.944465	0.492130	1.331266
14	6	0	2.732756	2.258798	-0.961389
15	1	0	3.689302	1.833748	-0.658370
16	1	0	2.507477	1.952635	-1.991108
17	1	0	2.812510	3.345890	-0.937499
18	6	0	2.651156	-0.457981	0.388555
19	6	0	2.959783	-1.139309	1.579939
20	6	0	3.329098	-0.815920	-0.791868
21	6	0	3.947786	-2.122041	1.601264
22	1	0	2.428868	-0.886268	2.492867
23	6	0	4.309454	-1.804645	-0.768505
24	1	0	3.073562	-0.341774	-1.732798
25	6	0	4.626529	-2.455403	0.427506
26	1	0	4.182583	-2.629721	2.531476
27	1	0	4.821242	-2.073958	-1.687036
28	1	0	5.391645	-3.225453	0.440738
29	6	0	-0.617304	0.290845	-0.850247
30	6	0	-1.571689	-0.661967	-0.351042
31	1	0	-0.408790	0.107735	-1.908091
32	1	0	0.540384	0.023254	-0.358142
33	6	0	-1.842124	-1.791913	-1.230588
34	8	0	-1.382874	-1.908807	-2.369598
35	8	0	-2.643908	-2.755246	-0.701930
36	6	0	-2.017111	-0.506749	1.026364
37	8	0	-1.424657	0.187947	1.856807
38	8	0	-3.168998	-1.149189	1.350059
39	6	0	-2.916730	-3.868342	-1.563566
40	1	0	-1.996617	-4.395405	-1.829442
41	1	0	-3.574162	-4.525404	-0.993749
42	1	0	-3.413215	-3.543879	-2.481827
43	6	0	-3.586907	-1.013927	2.716035
44	1	0	-4.493622	-1.612378	2.805693
45	1	0	-2.820063	-1.385791	3.400537
46	1	0	-3.799439	0.030217	2.959963

0903aab_Ph_NMeBn_CHC_COOMe_COOMe_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.829174	3.530693	1.053571
2	6	0	-1.925998	2.374039	0.287049
3	6	0	-0.791358	1.670900	-0.157078
4	6	0	0.451961	2.206591	0.215119
5	6	0	0.569698	3.367480	0.989828
6	6	0	-0.574680	4.031517	1.415401
7	1	0	-2.731664	4.044928	1.370255
8	1	0	-2.898718	1.991278	-0.003751
9	1	0	1.553892	3.731942	1.266294
10	1	0	-0.487651	4.926569	2.022552
11	7	0	1.702915	1.591383	-0.220402
12	6	0	1.996682	0.394138	0.207613
13	1	0	1.202598	-0.081216	0.788853
14	6	0	2.518529	2.386674	-1.159001
15	1	0	3.229698	3.012216	-0.614687
16	1	0	3.052039	1.720646	-1.835860
17	1	0	1.843993	3.024317	-1.727328
18	6	0	3.166772	-0.421084	-0.048271
19	6	0	2.962685	-1.809111	0.134400
20	6	0	4.453065	0.046976	-0.397771
21	6	0	4.002801	-2.705751	-0.080529
22	1	0	1.976215	-2.156818	0.427302
23	6	0	5.491521	-0.858319	-0.584235
24	1	0	4.660437	1.105668	-0.478036
25	6	0	5.267055	-2.231643	-0.440690
26	1	0	3.833814	-3.770208	0.043338
27	1	0	6.481052	-0.492901	-0.837417
28	1	0	6.083334	-2.930052	-0.596317
29	6	0	-0.995067	0.430176	-1.022149
30	6	0	-1.945501	-0.606549	-0.445106
31	1	0	-1.421036	0.771450	-1.970884
32	1	0	-0.032383	-0.030360	-1.255088
33	6	0	-3.278027	-0.578398	-0.966072
34	8	0	-3.701185	0.261489	-1.782072
35	8	0	-4.131663	-1.562774	-0.518516
36	6	0	-1.405292	-1.463904	0.547863
37	8	0	-0.230642	-1.395587	0.985458
38	8	0	-2.233724	-2.433238	1.062048
39	6	0	-5.459972	-1.497048	-1.038428
40	1	0	-5.473488	-1.605039	-2.127262
41	1	0	-5.998755	-2.327742	-0.578696
42	1	0	-5.947493	-0.551572	-0.781613
43	6	0	-1.657512	-3.268008	2.067350
44	1	0	-2.455873	-3.942898	2.381590
45	1	0	-0.816420	-3.849736	1.677289
46	1	0	-1.305423	-2.685486	2.923749

0911aaa_Ph_NMeBn_CHC_COOMe_COOMe_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.755539	-0.329767	0.448257
2	6	0	-3.736694	0.597436	0.671529
3	6	0	-2.394133	0.217412	0.709788
4	6	0	-2.038677	-1.134926	0.480668
5	6	0	-3.075003	-2.066716	0.255066
6	6	0	-4.409476	-1.666134	0.244023
7	1	0	-5.793997	-0.014746	0.433450
8	1	0	-3.982425	1.643685	0.837929
9	1	0	-2.836359	-3.107697	0.073297
10	1	0	-5.181245	-2.409832	0.065731
11	7	0	-0.703651	-1.546787	0.470595
12	6	0	0.385353	-0.584721	0.684859
13	1	0	0.546791	-0.447308	1.765153
14	6	0	-0.430465	-2.938026	0.837411
15	1	0	0.614828	-3.042765	1.122986
16	1	0	-1.052223	-3.250790	1.685351
17	1	0	-0.614323	-3.625730	0.003948

18	6	0	1.726381	-1.071861	0.129049
19	6	0	2.878779	-0.869594	0.902110
20	6	0	1.854834	-1.727330	-1.103932
21	6	0	4.133430	-1.280193	0.446160
22	1	0	2.794289	-0.392551	1.875021
23	6	0	3.105755	-2.147723	-1.555836
24	1	0	0.971443	-1.898290	-1.704653
25	6	0	4.250739	-1.920967	-0.787370
26	1	0	5.012178	-1.110282	1.061221
27	1	0	3.186234	-2.655913	-2.512551
28	1	0	5.222650	-2.249675	-1.143421
29	6	0	-1.309501	1.224545	1.002456
30	6	0	-0.036490	0.852602	0.200737
31	1	0	-1.639211	2.232731	0.744291
32	1	0	-1.051296	1.231143	2.066089
33	6	0	1.122294	1.818390	0.482239
34	8	0	1.845445	2.291819	-0.370644
35	8	0	1.258941	2.056782	1.795073
36	6	0	-0.359460	0.963753	-1.303378
37	8	0	-0.245408	0.096039	-2.141353
38	8	0	-0.834839	2.191302	-1.578101
39	6	0	2.346823	2.932263	2.169726
40	1	0	2.296882	3.008663	3.254238
41	1	0	3.300486	2.503555	1.856704
42	1	0	2.217068	3.912455	1.707749
43	6	0	-1.174906	2.442213	-2.956964
44	1	0	-1.952029	1.751014	-3.289095
45	1	0	-1.538090	3.468135	-2.985359
46	1	0	-0.293487	2.330241	-3.591627

1001aab_Ph_NMeBn_CHC_COOMe_H_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.541779	0.291263	0.211397
2	6	0	3.344909	0.994622	0.144653
3	6	0	2.110576	0.342917	-0.035863
4	6	0	2.087902	-1.080992	-0.117973
5	6	0	3.310124	-1.774664	-0.068750
6	6	0	4.518718	-1.099984	0.089820
7	1	0	5.481203	0.820627	0.333427
8	1	0	3.360950	2.079220	0.182810
9	1	0	3.318801	-2.855800	-0.132067
10	1	0	5.443648	-1.667921	0.129469
11	7	0	0.856522	-1.763755	-0.270813
12	6	0	-0.106170	-1.637664	0.836062
13	1	0	0.054620	-0.671566	1.322237
14	1	0	0.099362	-2.402290	1.604226
15	6	0	0.922519	-3.132050	-0.781963
16	1	0	-0.083945	-3.448128	-1.063663
17	1	0	1.554698	-3.170294	-1.671371
18	1	0	1.306314	-3.852180	-0.041598
19	6	0	-1.564501	-1.740551	0.417701
20	6	0	-2.518041	-2.134493	1.366632
21	6	0	-1.998854	-1.407460	-0.871168
22	6	0	-3.874257	-2.179424	1.041927
23	1	0	-2.194830	-2.407221	2.368523
24	6	0	-3.355380	-1.459400	-1.201444
25	1	0	-1.266779	-1.122843	-1.620255
26	6	0	-4.298411	-1.841360	-0.245810
27	1	0	-4.598231	-2.485732	1.791546
28	1	0	-3.673455	-1.202146	-2.207767
29	1	0	-5.352820	-1.881841	-0.502636
30	6	0	0.884335	1.114887	-0.225920
31	6	0	0.648936	2.376280	0.188301
32	1	0	0.085610	0.618746	-0.771463
33	6	0	-0.620390	3.046665	-0.139306
34	8	0	-1.541460	2.573982	-0.788880
35	8	0	-0.653620	4.295062	0.384488
36	6	0	-1.851389	5.048729	0.127710
37	1	0	-1.702629	6.013090	0.611740
38	1	0	-2.000103	5.181395	-0.946517

39	1	0	-2.723011	4.542384	0.549094
40	1	0	1.361159	2.942521	0.779063

1002dab_Ph_NMeBn_CHC_COOMe_H_ZWion_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.195403	-3.479360	-0.661900
2	6	0	-2.271410	-2.086311	-0.622089
3	6	0	-1.181913	-1.297459	-0.235200
4	6	0	-0.009974	-1.988392	0.112413
5	6	0	0.091640	-3.378904	0.087629
6	6	0	-1.013619	-4.132310	-0.307112
7	1	0	-3.061931	-4.057115	-0.970150
8	1	0	-3.190640	-1.566890	-0.877710
9	1	0	1.023272	-3.858523	0.371124
10	1	0	-0.947372	-5.214952	-0.337813
11	7	0	1.147609	-1.219586	0.562037
12	6	0	1.807166	-0.534140	-0.341350
13	1	0	1.441781	-0.693663	-1.351009
14	6	0	1.402042	-1.189078	2.013942
15	1	0	2.332507	-1.712137	2.246210
16	1	0	1.453039	-0.156752	2.365042
17	1	0	0.576594	-1.695633	2.507924
18	6	0	2.931520	0.365086	-0.230695
19	6	0	3.264683	1.040527	-1.431133
20	6	0	3.716707	0.608834	0.921837
21	6	0	4.320452	1.940126	-1.475035
22	1	0	2.677833	0.855001	-2.325401
23	6	0	4.777589	1.504285	0.864352
24	1	0	3.526094	0.095578	1.852154
25	6	0	5.079456	2.175437	-0.325034
26	1	0	4.555213	2.453493	-2.401206
27	1	0	5.375564	1.678331	1.752506
28	1	0	5.908797	2.874805	-0.355864
29	6	0	-1.281019	0.230105	-0.174234
30	6	0	-2.546829	0.846554	-0.664787
31	1	0	-1.144906	0.543066	0.870476
32	1	0	-0.389086	0.629053	-0.702606
33	6	0	-3.265203	1.725067	0.137067
34	8	0	-3.053436	2.075992	1.324402
35	8	0	-4.389998	2.266656	-0.536125
36	6	0	-5.203342	3.125572	0.245909
37	1	0	-4.644661	3.983037	0.638249
38	1	0	-5.996493	3.483845	-0.416288
39	1	0	-5.657308	2.606605	1.099607
40	1	0	-2.859342	0.694930	-1.693212

1003aab_Ph_NMeBn_CHC_COOMe_H_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.879942	3.387368	-0.468451
2	6	0	2.202932	2.041586	-0.296282
3	6	0	1.239708	1.082031	0.041025
4	6	0	-0.076359	1.552706	0.187911
5	6	0	-0.425662	2.894289	0.009331
6	6	0	0.560839	3.820754	-0.321396
7	1	0	2.658605	4.099144	-0.726838
8	1	0	3.218368	1.688039	-0.446561
9	1	0	-1.457997	3.202691	0.142320
10	1	0	0.298357	4.864133	-0.462304
11	7	0	-1.149282	0.632564	0.553806
12	6	0	-2.078665	0.380427	-0.332204
13	1	0	-1.855902	0.781795	-1.316709
14	6	0	-1.149038	0.144812	1.945837
15	1	0	-1.766295	0.800009	2.565885
16	1	0	-1.520089	-0.878561	1.983576

17	1	0	-0.125975	0.175989	2.311968
18	6	0	-3.314761	-0.358804	-0.223535
19	6	0	-3.889029	-0.739945	-1.460106
20	6	0	-3.994506	-0.686865	0.973158
21	6	0	-5.074175	-1.462117	-1.500098
22	1	0	-3.388098	-0.471982	-2.385046
23	6	0	-5.189886	-1.392840	0.920835
24	1	0	-3.623007	-0.365394	1.935433
25	6	0	-5.725726	-1.791634	-0.308374
26	1	0	-5.494901	-1.758891	-2.454673
27	1	0	-5.710174	-1.629677	1.842616
28	1	0	-6.657252	-2.347819	-0.336209
29	6	0	1.620074	-0.389359	0.221565
30	6	0	2.785404	-0.876565	-0.580254
31	1	0	1.880910	-0.545753	1.278793
32	1	0	0.703896	-0.981337	0.053491
33	6	0	3.917423	-1.373218	0.045613
34	8	0	4.175738	-1.481138	1.272767
35	8	0	4.895104	-1.821742	-0.887365
36	6	0	6.096172	-2.306141	-0.313187
37	1	0	5.923874	-3.146802	0.369170
38	1	0	6.721579	-2.641604	-1.145805
39	1	0	6.635317	-1.531361	0.247189
40	1	0	2.728888	-0.876444	-1.664462

1011aaa_Ph_NMeBn_CHC_COOMe_H_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.847815	0.266603	-0.420459
2	6	0	-3.764660	1.146617	-0.447489
3	6	0	-2.470189	0.733035	-0.129860
4	6	0	-2.227959	-0.623481	0.201398
5	6	0	-3.329686	-1.507292	0.230408
6	6	0	-4.615450	-1.064491	-0.074399
7	1	0	-5.847092	0.613791	-0.663275
8	1	0	-3.922319	2.190586	-0.709144
9	1	0	-3.181985	-2.550339	0.481456
10	1	0	-5.437747	-1.774113	-0.043589
11	7	0	-0.940038	-1.090640	0.480601
12	6	0	0.217679	-0.183934	0.508301
13	1	0	0.346573	0.240824	1.515504
14	6	0	-0.820786	-2.311072	1.276946
15	1	0	0.210310	-2.427351	1.607225
16	1	0	-1.467297	-2.278115	2.163953
17	1	0	-1.081088	-3.202951	0.696018
18	6	0	1.505980	-0.917127	0.140930
19	6	0	2.654902	-0.760181	0.925062
20	6	0	1.575709	-1.717124	-1.008840
21	6	0	3.853530	-1.383226	0.566383
22	1	0	2.611021	-0.148338	1.822000
23	6	0	2.769633	-2.341962	-1.366845
24	1	0	0.685132	-1.858265	-1.614500
25	6	0	3.913895	-2.175220	-0.580649
26	1	0	4.735192	-1.253167	1.187065
27	1	0	2.808110	-2.960693	-2.258705
28	1	0	4.842994	-2.663525	-0.859238
29	6	0	-1.327014	1.716791	-0.119465
30	6	0	-0.013153	0.998826	-0.467028
31	1	0	-1.516076	2.525878	-0.832960
32	1	0	-1.224070	2.184992	0.867769
33	6	0	1.159081	1.964735	-0.471285
34	8	0	1.794896	2.279214	-1.458332
35	8	0	1.397861	2.466280	0.755991
36	6	0	2.484896	3.409763	0.854271
37	1	0	2.522533	3.705086	1.901533
38	1	0	3.423698	2.939156	0.555377
39	1	0	2.295052	4.276735	0.218414
40	1	0	-0.076303	0.602768	-1.484655

1101aab_Ph_NMeBn_CHC_NO2_NO2_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.817776	1.865704	-0.163501
2	6	0	-3.062819	0.707329	-0.192139
3	6	0	-1.649101	0.753354	-0.217555
4	6	0	-0.984645	2.020123	-0.148765
5	6	0	-1.777755	3.185216	-0.149407
6	6	0	-3.164122	3.106259	-0.154242
7	1	0	-4.900749	1.812826	-0.174596
8	1	0	-3.567954	-0.247797	-0.278946
9	1	0	-1.307070	4.158702	-0.106638
10	1	0	-3.745019	4.023341	-0.134419
11	7	0	0.410580	2.085897	-0.102147
12	6	0	1.127476	1.352928	0.956497
13	1	0	0.458382	0.594510	1.370861
14	1	0	1.344055	2.046232	1.784199
15	6	0	1.041263	3.370962	-0.410835
16	1	0	2.107445	3.202215	-0.569985
17	1	0	0.620612	3.788015	-1.327239
18	1	0	0.928996	4.101155	0.403730
19	6	0	2.426484	0.695721	0.515226
20	6	0	3.326116	0.265112	1.501223
21	6	0	2.746817	0.476064	-0.828888
22	6	0	4.509664	-0.383832	1.152320
23	1	0	3.095698	0.438235	2.549771
24	6	0	3.936594	-0.168422	-1.181099
25	1	0	2.070222	0.822047	-1.604139
26	6	0	4.819675	-0.603435	-0.193192
27	1	0	5.192875	-0.713089	1.929747
28	1	0	4.170504	-0.326571	-2.229846
29	1	0	5.743685	-1.104010	-0.466516
30	6	0	-0.866152	-0.428716	-0.479244
31	6	0	-1.139919	-1.723951	-0.204342
32	1	0	0.073337	-0.283351	-1.005993
33	7	0	-0.277796	-2.794274	-0.642019
34	8	0	-0.454186	-3.909664	-0.141623
35	8	0	0.604326	-2.525645	-1.462091
36	7	0	-2.269309	-2.181814	0.613706
37	8	0	-3.076509	-2.944197	0.087985
38	8	0	-2.343649	-1.748447	1.760838

1102dab_Ph_NMeBn_CHC_NO2_NO2_ZWion_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.295143	-0.852351	-0.711544
2	6	0	3.261138	0.023326	-1.039271
3	6	0	1.934646	-0.261382	-0.691506
4	6	0	1.606976	-1.476182	-0.031901
5	6	0	2.670440	-2.338420	0.295289
6	6	0	3.989575	-2.029386	-0.031298
7	1	0	5.318760	-0.608915	-0.975377
8	1	0	3.481516	0.955590	-1.550500
9	1	0	2.462224	-3.272579	0.801745
10	1	0	4.778188	-2.726015	0.237083
11	7	0	0.277439	-1.772754	0.329636
12	6	0	-0.735047	-1.825357	-0.731470
13	1	0	-0.384628	-1.235731	-1.583289
14	6	0	0.072419	-2.805002	1.341803
15	1	0	-0.965111	-2.756779	1.678999
16	1	0	0.258899	-3.823725	0.965926
17	1	0	0.718918	-2.622328	2.202584
18	6	0	-2.107387	-1.323802	-0.309551
19	6	0	-2.265933	-0.370119	0.703540
20	6	0	-3.245153	-1.792364	-0.979944
21	6	0	-3.535673	0.110465	1.032757
22	1	0	-1.389812	-0.016835	1.238225
23	6	0	-4.513456	-1.307814	-0.657401

24	1	0	-3.136860	-2.541831	-1.760421
25	6	0	-4.662916	-0.353238	0.351840
26	1	0	-3.642874	0.847837	1.823272
27	1	0	-5.384562	-1.681254	-1.188009
28	1	0	-5.649663	0.020721	0.608567
29	6	0	0.919260	0.765279	-1.036372
30	6	0	0.549174	1.779885	-0.254745
31	1	0	0.467674	0.774955	-2.027269
32	1	0	-0.829950	-2.855188	-1.114097
33	7	0	-0.442219	2.774689	-0.676347
34	8	0	-0.773895	2.777946	-1.857690
35	8	0	-0.897534	3.510496	0.195375
36	7	0	1.102809	2.042110	1.082037
37	8	0	0.977915	1.171292	1.935614
38	8	0	1.684996	3.111833	1.225942

1103aab_Ph_NMeBn_CHC_NO2_NO2_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.747807	2.877069	0.984060
2	6	0	-2.719031	1.698981	0.241478
3	6	0	-1.514381	1.159975	-0.237523
4	6	0	-0.342894	1.864315	0.071517
5	6	0	-0.351355	3.046532	0.815908
6	6	0	-1.562354	3.555799	1.276389
7	1	0	-3.697802	3.266953	1.336144
8	1	0	-3.640259	1.173648	0.011679
9	1	0	0.584930	3.550678	1.032044
10	1	0	-1.577372	4.471144	1.858519
11	7	0	0.953209	1.386398	-0.402546
12	6	0	1.606934	0.540031	0.343433
13	1	0	1.049385	0.196690	1.207473
14	6	0	1.400080	1.913139	-1.705999
15	1	0	1.905122	2.872000	-1.568093
16	1	0	2.067587	1.200121	-2.186858
17	1	0	0.515242	2.065692	-2.322492
18	6	0	2.923741	-0.032334	0.154831
19	6	0	3.129341	-1.287119	0.771506
20	6	0	3.991623	0.586790	-0.530207
21	6	0	4.356900	-1.928714	0.660594
22	1	0	2.306576	-1.756876	1.300800
23	6	0	5.223863	-0.052108	-0.609505
24	1	0	3.882755	1.576648	-0.954065
25	6	0	5.404891	-1.311203	-0.028083
26	1	0	4.501891	-2.901365	1.118277
27	1	0	6.047287	0.434471	-1.121090
28	1	0	6.368593	-1.805077	-0.101914
29	6	0	-1.532347	-0.124816	-1.059049
30	6	0	-2.151641	-1.303116	-0.361775
31	1	0	-2.113282	0.054973	-1.965653
32	1	0	-0.519690	-0.398686	-1.355893
33	7	0	-3.483912	-1.626468	-0.613103
34	8	0	-4.134197	-0.822048	-1.343551
35	8	0	-4.027313	-2.652807	-0.157006
36	7	0	-1.375370	-2.042564	0.515657
37	8	0	-0.181412	-1.632092	0.682825
38	8	0	-1.786057	-3.048292	1.128434

1111aaa_Ph_NMeBn_CHC_NO2_NO2_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.691292	-0.626211	-0.540739
2	6	0	3.759395	0.359736	-0.855006
3	6	0	2.394741	0.186031	-0.604088
4	6	0	1.942927	-1.021414	-0.014534
5	6	0	2.896748	-2.005832	0.323032

6	6	0	4.247503	-1.808141	0.058213
7	1	0	5.744955	-0.470689	-0.747740
8	1	0	4.091015	1.296231	-1.296307
9	1	0	2.574663	-2.933490	0.779848
10	1	0	4.957033	-2.587380	0.320728
11	7	0	0.587947	-1.213783	0.253172
12	6	0	-0.355095	-0.336048	-0.423817
13	1	0	-0.181417	-0.429081	-1.503493
14	6	0	0.173015	-2.224675	1.216708
15	1	0	-0.863070	-2.057686	1.499032
16	1	0	0.256198	-3.239384	0.806792
17	1	0	0.788168	-2.162177	2.120008
18	6	0	-1.831022	-0.676432	-0.249311
19	6	0	-2.381596	-1.541810	-1.208583
20	6	0	-2.661816	-0.192926	0.771724
21	6	0	-3.719990	-1.925708	-1.147215
22	1	0	-1.753364	-1.918136	-2.011400
23	6	0	-4.005916	-0.568824	0.825856
24	1	0	-2.269592	0.472297	1.528617
25	6	0	-4.538736	-1.436670	-0.127506
26	1	0	-4.122588	-2.597385	-1.899030
27	1	0	-4.634918	-0.180358	1.620938
28	1	0	-5.583853	-1.726719	-0.078993
29	6	0	1.441493	1.319675	-0.927810
30	6	0	0.117068	1.149531	-0.186373
31	1	0	1.882622	2.285362	-0.672831
32	1	0	1.190613	1.345401	-1.992223
33	7	0	0.312407	1.538187	1.292153
34	8	0	-0.131737	0.798775	2.160458
35	8	0	0.921641	2.579354	1.499197
36	7	0	-0.925486	2.107829	-0.723627
37	8	0	-1.569888	2.786137	0.069282
38	8	0	-1.085094	2.082719	-1.940079

1201aab_Ph_NMeBn_CHC_NO2_H_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.436755	-0.366993	0.202385
2	6	0	3.414184	0.569233	0.179020
3	6	0	2.067298	0.189561	0.000437
4	6	0	1.743793	-1.197859	-0.111401
5	6	0	2.799789	-2.128471	-0.112812
6	6	0	4.121215	-1.720251	0.039511
7	1	0	5.467262	-0.049859	0.321593
8	1	0	3.657076	1.624649	0.245736
9	1	0	2.585826	-3.185859	-0.203358
10	1	0	4.909189	-2.467496	0.045683
11	7	0	0.402521	-1.609084	-0.241627
12	6	0	-0.520227	-1.277033	0.857682
13	1	0	-0.134933	-0.397177	1.379700
14	1	0	-0.519479	-2.092118	1.599963
15	6	0	0.167136	-2.954845	-0.765257
16	1	0	-0.888406	-3.044873	-1.028455
17	1	0	0.759536	-3.116497	-1.667750
18	1	0	0.402392	-3.745379	-0.035940
19	6	0	-1.952897	-1.009897	0.422948
20	6	0	-2.978342	-1.116153	1.373191
21	6	0	-2.283070	-0.620101	-0.880292
22	6	0	-4.299501	-0.824705	1.033999
23	1	0	-2.738896	-1.428780	2.386854
24	6	0	-3.607137	-0.334623	-1.224511
25	1	0	-1.501058	-0.555290	-1.630374
26	6	0	-4.619084	-0.431979	-0.268724
27	1	0	-5.080146	-0.910878	1.784283
28	1	0	-3.845281	-0.038014	-2.241938
29	1	0	-5.648034	-0.210601	-0.536135
30	6	0	1.033697	1.194382	-0.175697
31	6	0	1.098820	2.479469	0.224193
32	1	0	0.129516	0.888248	-0.692785
33	7	0	0.035971	3.396274	-0.078657
34	8	0	0.158068	4.548946	0.364959

35	8	0	-0.938920	3.022984	-0.745967
36	1	0	1.888239	2.945744	0.794948

1202dab_Ph_NMeBn_CHC_NO2_H_ZWion_B3lyp631pd_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.351974	-0.778555	0.188136
2	6	0	3.404187	0.220502	-0.046696
3	6	0	2.038623	-0.072063	-0.101389
4	6	0	1.640673	-1.415414	0.075166
5	6	0	2.583252	-2.416002	0.314553
6	6	0	3.941061	-2.098736	0.366696
7	1	0	5.405007	-0.520734	0.239351
8	1	0	3.720132	1.249310	-0.190612
9	1	0	2.251738	-3.437267	0.471580
10	1	0	4.668953	-2.880632	0.557569
11	7	0	0.244828	-1.740131	-0.019646
12	6	0	-0.579582	-0.781746	0.517528
13	1	0	-0.253344	-0.470307	1.512471
14	6	0	-0.156697	-2.641310	-1.105176
15	1	0	-1.178569	-2.980051	-0.938582
16	1	0	-0.083600	-2.165505	-2.090521
17	1	0	0.503644	-3.508711	-1.093642
18	6	0	-2.036535	-0.701824	0.310317
19	6	0	-2.841147	-0.480313	1.444450
20	6	0	-2.650663	-0.758013	-0.956410
21	6	0	-4.223326	-0.359281	1.322105
22	1	0	-2.377547	-0.416259	2.424346
23	6	0	-4.031453	-0.627491	-1.074087
24	1	0	-2.050318	-0.874619	-1.851098
25	6	0	-4.822269	-0.435168	0.062869
26	1	0	-4.830536	-0.201597	2.207714
27	1	0	-4.491198	-0.667638	-2.056385
28	1	0	-5.898725	-0.335096	-0.034938
29	6	0	1.029592	1.015089	-0.391414
30	6	0	1.178817	2.248817	0.301656
31	1	0	0.789752	1.145815	-1.452251
32	1	0	-0.046030	0.453017	-0.048345
33	7	0	0.525269	3.377834	-0.131704
34	8	0	-0.207953	3.329688	-1.161499
35	8	0	0.685549	4.455070	0.510477
36	1	0	1.700141	2.357335	1.241153

1203aab_Ph_NMeBn_CHC_NO2_H_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.883251	2.539213	-0.726573
2	6	0	2.913014	1.245515	-0.210903
3	6	0	1.742166	0.592260	0.207541
4	6	0	0.544547	1.311578	0.083086
5	6	0	0.492876	2.606732	-0.444630
6	6	0	1.671070	3.223729	-0.853721
7	1	0	3.808691	3.016254	-1.035125
8	1	0	3.848235	0.702717	-0.109983
9	1	0	-0.460599	3.120233	-0.516405
10	1	0	1.641424	4.229060	-1.260661
11	7	0	-0.716140	0.727032	0.531750
12	6	0	-1.590185	0.367183	-0.369915
13	1	0	-1.212587	0.426297	-1.386970
14	6	0	-0.920325	0.657563	1.991669
15	1	0	-1.426709	1.562467	2.336248
16	1	0	-1.502555	-0.226938	2.246698
17	1	0	0.058120	0.602251	2.463213
18	6	0	-2.945860	-0.113090	-0.230816
19	6	0	-3.460171	-0.778040	-1.368964
20	6	0	-3.781393	0.060094	0.897031

21	6	0	-4.747776	-1.297849	-1.363560
22	1	0	-2.834310	-0.892137	-2.248415
23	6	0	-5.075687	-0.444281	0.883306
24	1	0	-3.448505	0.617214	1.761230
25	6	0	-5.556349	-1.132724	-0.235801
26	1	0	-5.124753	-1.819008	-2.236694
27	1	0	-5.715686	-0.296393	1.746322
28	1	0	-6.567034	-1.528129	-0.232281
29	6	0	1.824830	-0.840843	0.730040
30	6	0	2.560800	-1.791060	-0.163928
31	1	0	2.333056	-0.819906	1.701960
32	1	0	0.815233	-1.230348	0.896227
33	7	0	3.871765	-1.992973	-0.039230
34	8	0	4.563748	-1.326413	0.832859
35	8	0	4.474457	-2.857577	-0.780788
36	1	0	2.064111	-2.366018	-0.932750

1211aaa_Ph_NMeBn_CHC_NO2_H_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.715686	-0.058696	-0.430343
2	6	0	-3.747253	0.940683	-0.340949
3	6	0	-2.414117	0.647608	-0.047676
4	6	0	-2.011388	-0.698122	0.132818
5	6	0	-2.999556	-1.703339	0.045620
6	6	0	-4.326956	-1.383596	-0.230035
7	1	0	-5.748325	0.192455	-0.649827
8	1	0	-4.026779	1.981238	-0.487324
9	1	0	-2.730768	-2.742934	0.182774
10	1	0	-5.058782	-2.184108	-0.291638
11	7	0	-0.672932	-1.039513	0.365011
12	6	0	0.350554	-0.005795	0.562082
13	1	0	0.380992	0.326498	1.610914
14	6	0	-0.404158	-2.335011	0.991032
15	1	0	0.642551	-2.384143	1.284982
16	1	0	-1.024141	-2.486434	1.884397
17	1	0	-0.589773	-3.160918	0.296732
18	6	0	1.741220	-0.500985	0.175663
19	6	0	2.824147	-0.293064	1.036995
20	6	0	1.964005	-1.123927	-1.060892
21	6	0	4.110748	-0.696677	0.670082
22	1	0	2.661087	0.185391	1.998805
23	6	0	3.246693	-1.529001	-1.426820
24	1	0	1.126165	-1.302981	-1.728674
25	6	0	4.324528	-1.314814	-0.562197
26	1	0	4.941431	-0.531195	1.349513
27	1	0	3.406143	-2.012901	-2.385821
28	1	0	5.323104	-1.631817	-0.847590
29	6	0	-1.406034	1.761055	0.097338
30	6	0	-0.028027	1.233283	-0.285644
31	1	0	-1.676100	2.610557	-0.537519
32	1	0	-1.361838	2.126078	1.130353
33	7	0	1.005988	2.308362	-0.060460
34	8	0	1.650919	2.698290	-1.030234
35	8	0	1.138550	2.738116	1.085821
36	1	0	0.035566	1.004404	-1.349092

1301aab_Ph_NMeBn_CHC_CF3_CF3_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.317126	2.809418	-0.202768
2	6	0	-2.796239	1.523112	-0.285970
3	6	0	-1.408455	1.298088	-0.316169
4	6	0	-0.519187	2.408002	-0.230626
5	6	0	-1.064741	3.701177	-0.158979
6	6	0	-2.443823	3.897892	-0.148709

7	1	0	-4.391289	2.962351	-0.201527
8	1	0	-3.468966	0.679863	-0.384160
9	1	0	-0.409616	4.560867	-0.090978
10	1	0	-2.835665	4.908894	-0.087333
11	7	0	0.876606	2.184898	-0.245247
12	6	0	1.433414	1.405946	0.874541
13	1	0	0.656095	0.731899	1.244270
14	1	0	1.674716	2.079157	1.713818
15	6	0	1.723163	3.326031	-0.593052
16	1	0	2.733010	2.962505	-0.793059
17	1	0	1.347649	3.809942	-1.496722
18	1	0	1.787087	4.074221	0.212483
19	6	0	2.669280	0.590322	0.528138
20	6	0	3.542402	0.215817	1.559096
21	6	0	2.945021	0.156999	-0.774274
22	6	0	4.654793	-0.584956	1.299146
23	1	0	3.348009	0.554160	2.574140
24	6	0	4.063217	-0.638014	-1.038887
25	1	0	2.291325	0.459991	-1.585793
26	6	0	4.919495	-1.015742	-0.003524
27	1	0	5.318491	-0.865805	2.111818
28	1	0	4.264064	-0.960218	-2.056631
29	1	0	5.788324	-1.633855	-0.209381
30	6	0	-0.849550	-0.022988	-0.607153
31	6	0	-1.232915	-1.255230	-0.217594
32	1	0	0.020134	0.012062	-1.257502
33	6	0	-2.327968	-1.550043	0.774591
34	6	0	-0.531418	-2.466868	-0.774557
35	9	0	0.210550	-3.110821	0.156720
36	9	0	-1.420706	-3.371043	-1.254788
37	9	0	-2.146180	-2.747711	1.373167
38	9	0	-3.556704	-1.595002	0.193888
39	9	0	-2.391779	-0.624966	1.754026
40	9	0	0.303064	-2.153136	-1.787037

1302dab_Ph_NMeBn_CHC_CF3_CF3_ZW_INT_B3lyp631pd_PCMdmso_TS_CH_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.624653	3.082565	0.796541
2	6	0	-2.529940	1.930606	0.023311
3	6	0	-1.291308	1.408883	-0.393271
4	6	0	-0.154162	2.119024	0.018240
5	6	0	-0.226986	3.279374	0.798602
6	6	0	-1.468633	3.763432	1.192747
7	1	0	-3.601300	3.454168	1.091766
8	1	0	-3.431845	1.405035	-0.269909
9	1	0	0.686410	3.784362	1.097455
10	1	0	-1.533025	4.657743	1.803639
11	7	0	1.185611	1.685792	-0.378881
12	6	0	1.737778	0.695069	0.268143
13	1	0	1.122366	0.302898	1.071947
14	6	0	1.823363	2.461615	-1.459966
15	1	0	1.671385	1.958621	-2.418241
16	1	0	1.345328	3.438089	-1.494573
17	1	0	2.887052	2.581644	-1.258288
18	6	0	3.020681	0.051592	0.086709
19	6	0	3.436735	-0.744868	1.179019
20	6	0	3.841754	0.116608	-1.062052
21	6	0	4.655563	-1.409597	1.149161
22	1	0	2.795375	-0.828501	2.050427
23	6	0	5.050114	-0.569528	-1.090640
24	1	0	3.532461	0.660047	-1.943480
25	6	0	5.465612	-1.320163	0.013928
26	1	0	4.968363	-2.004907	2.000088
27	1	0	5.669092	-0.523755	-1.980142
28	1	0	6.414213	-1.846617	-0.017299
29	6	0	-1.255672	0.141938	-1.253586
30	6	0	-1.711719	-1.144887	-0.587826
31	1	0	-1.892177	0.328786	-2.123827
32	6	0	-0.824077	-1.729336	0.369207
33	6	0	-3.124589	-1.424295	-0.477071

34	9	0	-3.465906	-2.757269	-0.510835
35	9	0	-3.793369	-0.992422	0.692835
36	9	0	-1.210474	-2.936366	0.860801
37	9	0	-0.553242	-0.978476	1.573634
38	9	0	0.470886	-1.888445	-0.106661
39	9	0	-3.848628	-0.827207	-1.480081
40	1	0	-0.245545	0.005315	-1.651807

1303aab_Ph_NMeBn_CHC_CF3_CF3_ZW_INT_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.314718	2.812457	-0.202179
2	6	0	-2.795290	1.525563	-0.285601
3	6	0	-1.407781	1.299043	-0.316443
4	6	0	-0.517263	2.407974	-0.231280
5	6	0	-1.061330	3.701737	-0.159392
6	6	0	-2.440202	3.899968	-0.148525
7	1	0	-4.388712	2.966565	-0.200441
8	1	0	-3.468973	0.683029	-0.383416
9	1	0	-0.405218	4.560705	-0.091729
10	1	0	-2.830903	4.911402	-0.086998
11	7	0	0.878285	2.183173	-0.246463
12	6	0	1.434309	1.404102	0.873692
13	1	0	1.675166	2.077185	1.713203
14	6	0	1.725968	3.323365	-0.594652
15	1	0	2.735355	2.958738	-0.794947
16	1	0	1.350647	3.807564	-1.498250
17	1	0	1.790945	4.071589	0.210769
18	6	0	2.670222	0.588332	0.527905
19	6	0	3.543995	0.215512	1.558892
20	6	0	2.945245	0.153065	-0.774035
21	6	0	4.656339	-0.585539	1.299494
22	1	0	3.350178	0.555381	2.573534
23	6	0	4.063369	-0.642193	-1.038105
24	1	0	2.291073	0.454793	-1.585640
25	6	0	4.920312	-1.018262	-0.002662
26	1	0	5.320560	-0.865048	2.112201
27	1	0	4.263662	-0.965923	-2.055475
28	1	0	5.789087	-1.636586	-0.208110
29	6	0	-0.850367	-0.022617	-0.607673
30	6	0	-1.234487	-1.254436	-0.217543
31	1	0	0.018852	0.011547	-1.258695
32	6	0	-2.329183	-1.548007	0.775388
33	6	0	-0.534545	-2.466817	-0.774848
34	9	0	0.207261	-3.111472	0.156020
35	9	0	-1.425011	-3.370085	-1.254590
36	9	0	-2.148156	-2.745737	1.374132
37	9	0	-3.558311	-1.591939	0.195504
38	9	0	-2.391480	-0.622671	1.754715
39	9	0	0.299710	-2.153958	-1.787796
40	1	0	0.656619	0.730112	1.242770

1311aaa_Ph_NMeBn_CHC_CF3_CF3_product_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.374640	0.639936	0.770628
2	6	0	-3.532393	-0.467563	0.617735
3	6	0	-2.350810	-0.362096	-0.107884
4	6	0	-1.969871	0.874762	-0.667917
5	6	0	-2.815995	1.985855	-0.518317
6	6	0	-4.012925	1.856561	0.192216
7	1	0	-5.301415	0.548634	1.328080
8	1	0	-3.808201	-1.427691	1.046616
9	1	0	-2.545194	2.944712	-0.945573
10	1	0	-4.659107	2.723143	0.300219
11	7	0	-0.786582	0.890334	-1.412601

12	6	0	0.420654	0.174847	-0.954494
13	1	0	0.901665	-0.174330	-1.873063
14	6	0	-0.529875	2.003350	-2.314970
15	1	0	0.271105	1.723471	-3.004928
16	1	0	-1.429739	2.206213	-2.901129
17	1	0	-0.227116	2.929065	-1.805934
18	6	0	1.443321	1.109623	-0.288531
19	6	0	2.801441	0.979813	-0.607421
20	6	0	1.052115	2.146713	0.569566
21	6	0	3.751507	1.842466	-0.058921
22	1	0	3.120404	0.195922	-1.287375
23	6	0	1.999550	3.014539	1.113739
24	1	0	0.003396	2.282293	0.809537
25	6	0	3.353476	2.862795	0.806477
26	1	0	4.799697	1.722291	-0.316462
27	1	0	1.677445	3.813368	1.775292
28	1	0	4.089450	3.539964	1.229517
29	6	0	-1.442836	-1.518685	-0.409543
30	6	0	0.050270	-1.153421	-0.162749
31	1	0	-1.708441	-2.405197	0.167676
32	1	0	-1.530082	-1.774865	-1.471122
33	6	0	0.289375	-1.072427	1.365706
34	6	0	0.913326	-2.303629	-0.735269
35	9	0	1.593429	-0.976717	1.691541
36	9	0	-0.184224	-2.173177	1.993322
37	9	0	-0.343879	-0.016087	1.913003
38	9	0	0.653626	-3.479349	-0.129700
39	9	0	2.238264	-2.076373	-0.617623
40	9	0	0.662570	-2.473848	-2.053149

1313aab_Ph_NMeBn_CHC_CF3_CF3_ZWion_B3lyp631pd_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.143516	3.511717	0.841303
2	6	0	-2.246451	2.289302	0.187038
3	6	0	-1.115706	1.586766	-0.263837
4	6	0	0.126524	2.178902	-0.003344
5	6	0	0.255055	3.403897	0.663236
6	6	0	-0.886119	4.074965	1.086743
7	1	0	-3.042081	4.028216	1.165137
8	1	0	-3.218738	1.840469	0.010613
9	1	0	1.242398	3.812144	0.854429
10	1	0	-0.795071	5.022106	1.608121
11	7	0	1.371061	1.547153	-0.442391
12	6	0	1.831959	0.524651	0.223481
13	1	0	1.158077	0.159740	0.994105
14	6	0	2.006986	2.151246	-1.629017
15	1	0	2.621372	3.005450	-1.335002
16	1	0	2.616332	1.409158	-2.141967
17	1	0	1.210536	2.495729	-2.286972
18	6	0	3.078926	-0.194449	0.059858
19	6	0	3.074789	-1.532236	0.516254
20	6	0	4.276523	0.361486	-0.441683
21	6	0	4.224988	-2.306392	0.425254
22	1	0	2.154444	-1.956037	0.902253
23	6	0	5.427611	-0.415423	-0.502917
24	1	0	4.328082	1.402374	-0.732953
25	6	0	5.401745	-1.749294	-0.083228
26	1	0	4.209023	-3.338372	0.758952
27	1	0	6.349227	0.021197	-0.872414
28	1	0	6.303784	-2.350178	-0.141123
29	6	0	-1.311948	0.259985	-0.994849
30	6	0	-2.012586	-0.803889	-0.172002
31	1	0	-1.915598	0.474319	-1.882589
32	1	0	-0.348093	-0.093926	-1.379153
33	6	0	-1.195077	-1.584806	0.699264
34	6	0	-3.309321	-1.267349	-0.588479
35	9	0	-1.805640	-2.626176	1.313177
36	9	0	-0.030951	-2.151126	0.109612
37	9	0	-0.580672	-0.852936	1.746062
38	9	0	-4.090270	-1.805495	0.402050

39	9	0	-4.059751	-0.258993	-1.160405
40	9	0	-3.363538	-2.271599	-1.584179

1401_biphenylO_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.973223	2.114626	-2.424477
2	6	0	-0.597257	2.363676	-2.339110
3	6	0	0.161471	1.835558	-1.299099
4	6	0	-0.454793	1.043983	-0.326723
5	6	0	-1.854160	0.771747	-0.388746
6	6	0	-2.587290	1.329760	-1.462397
7	1	0	-2.556906	2.535707	-3.235530
8	1	0	-0.109030	2.975160	-3.091575
9	1	0	1.224503	2.030961	-1.236866
10	1	0	-3.652709	1.152854	-1.528780
11	8	0	0.227808	0.473670	0.708000
12	6	0	1.571616	0.816343	0.929647
13	6	0	2.608253	0.019439	0.381091
14	6	0	1.825778	1.925951	1.727669
15	6	0	3.926507	0.466554	0.645135
16	6	0	3.135696	2.326862	1.988753
17	1	0	0.977993	2.475193	2.125421
18	6	0	4.179873	1.591353	1.425901
19	1	0	4.763533	-0.086547	0.237985
20	1	0	3.331098	3.196017	2.607420
21	1	0	5.210469	1.885041	1.602924
22	6	0	3.480092	-1.805176	-1.048745
23	6	0	1.199521	-1.988081	-0.230152
24	6	0	2.793708	-2.982778	-1.742758
25	1	0	4.009260	-1.143630	-1.743286
26	1	0	4.213338	-2.170826	-0.311778
27	6	0	1.689403	-3.351980	-0.742940
28	1	0	0.883599	-2.028316	0.816298
29	1	0	3.486383	-3.802866	-1.947029
30	1	0	2.357935	-2.658391	-2.694191
31	1	0	0.880125	-3.938845	-1.184803
32	1	0	2.114706	-3.933612	0.082372
33	6	0	-2.427956	-0.027368	0.665244
34	6	0	-3.689635	-0.543531	0.825407
35	1	0	-1.742514	-0.264253	1.472042
36	6	0	-4.777072	-0.423196	-0.095327
37	7	0	-5.686328	-0.352983	-0.819700
38	6	0	-3.988359	-1.296364	2.007196
39	7	0	-4.239774	-1.909533	2.964604
40	7	0	2.369599	-1.095286	-0.400106
41	1	0	0.348232	-1.632662	-0.821619

1404_biphenylO_ZWINT_b3lyp631dp_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.249048	3.273379	-1.574628
2	6	0	1.031302	3.792279	-1.132148
3	6	0	0.147107	2.998842	-0.398408
4	6	0	0.496879	1.680621	-0.109380
5	6	0	1.709111	1.130304	-0.561232
6	6	0	2.575983	1.945667	-1.297823
7	1	0	2.934607	3.893614	-2.142729
8	1	0	0.762732	4.820512	-1.353436
9	1	0	-0.798052	3.403987	-0.059311
10	1	0	3.509351	1.527159	-1.663142
11	8	0	-0.282879	0.826309	0.658487
12	6	0	-1.655270	0.731485	0.523774
13	6	0	-2.180655	-0.435185	-0.069023
14	6	0	-2.507253	1.671142	1.102578
15	6	0	-3.568747	-0.625224	-0.075043

16	6	0	-3.888789	1.478351	1.071200
17	1	0	-2.079300	2.529330	1.607976
18	6	0	-4.417210	0.328540	0.483784
19	1	0	-3.983710	-1.517440	-0.530095
20	1	0	-4.544159	2.216135	1.521906
21	1	0	-5.489835	0.167586	0.461695
22	6	0	-1.559845	-2.878784	-0.372269
23	6	0	-0.287801	-1.206586	-1.454126
24	6	0	-0.322519	-3.538787	-0.998084
25	1	0	-1.672566	-3.067409	0.697617
26	1	0	-2.480903	-3.186537	-0.879360
27	6	0	0.119369	-2.525964	-2.071495
28	1	0	-0.299953	-0.280377	-2.026072
29	1	0	-0.550151	-4.522231	-1.411980
30	1	0	0.464163	-3.656886	-0.247349
31	1	0	1.181070	-2.576311	-2.319958
32	1	0	-0.447507	-2.657272	-3.002635
33	6	0	2.000322	-0.327362	-0.345812
34	6	0	2.362059	-0.816223	0.974141
35	1	0	2.649855	-0.731562	-1.126713
36	6	0	2.113564	-0.107413	2.166878
37	7	0	1.948677	0.472776	3.171414
38	6	0	2.929953	-2.101729	1.097636
39	7	0	3.396936	-3.173965	1.178579
40	7	0	-1.328999	-1.431349	-0.613718
41	1	0	0.911451	-0.849127	-0.711357

1405_biphenylO_ZWINT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.371461	-2.155548	1.691859
2	6	0	-2.128857	-2.290252	2.313509
3	6	0	-1.005214	-1.688902	1.745760
4	6	0	-1.142350	-0.963669	0.563872
5	6	0	-2.372845	-0.810312	-0.088886
6	6	0	-3.483121	-1.425523	0.507435
7	1	0	-4.251819	-2.619439	2.125991
8	1	0	-2.030859	-2.854630	3.235429
9	1	0	-0.028556	-1.771707	2.211809
10	1	0	-4.451070	-1.330346	0.022662
11	8	0	-0.019133	-0.299646	0.044272
12	6	0	1.009481	-1.036197	-0.475397
13	6	0	2.308809	-0.493947	-0.409177
14	6	0	0.822356	-2.277205	-1.091502
15	6	0	3.392045	-1.187669	-0.958596
16	6	0	1.905615	-2.956824	-1.642223
17	1	0	-0.175289	-2.698210	-1.134030
18	6	0	3.191871	-2.414569	-1.582174
19	1	0	4.386953	-0.760977	-0.904715
20	1	0	1.740466	-3.914587	-2.124739
21	1	0	4.034106	-2.942636	-2.014612
22	6	0	3.722148	0.882965	1.210996
23	6	0	1.822218	1.806093	0.237538
24	6	0	3.380540	2.152430	2.006256
25	1	0	3.812244	-0.020832	1.813387
26	1	0	4.617877	0.993722	0.595247
27	6	0	2.329362	2.875894	1.133705
28	1	0	0.976428	1.910484	-0.443052
29	1	0	4.265168	2.762716	2.188156
30	1	0	2.944415	1.883873	2.970676
31	1	0	1.513823	3.337677	1.697682
32	1	0	2.758542	3.668707	0.505148
33	6	0	-2.518038	-0.000151	-1.366039
34	6	0	-2.514440	1.513971	-1.156900
35	1	0	-3.446713	-0.313989	-1.858074
36	6	0	-1.393687	2.262462	-1.493456
37	7	0	-0.423019	2.866494	-1.793882
38	6	0	-3.603162	2.141638	-0.545677
39	7	0	-4.539627	2.644378	-0.037681
40	7	0	2.546013	0.733274	0.289657
41	1	0	-1.703836	-0.249792	-2.053214

1409_biphenylO_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.323049	-0.908739	-0.253432
2	6	0	4.349421	-0.037812	0.836371
3	6	0	3.177384	0.599303	1.245053
4	6	0	1.985549	0.362175	0.562255
5	6	0	1.928393	-0.523121	-0.529195
6	6	0	3.121439	-1.144041	-0.922907
7	1	0	5.230364	-1.406419	-0.580196
8	1	0	5.277414	0.150188	1.367235
9	1	0	3.167538	1.277625	2.091641
10	1	0	3.101480	-1.827615	-1.767208
11	8	0	0.829137	0.941546	1.064637
12	6	0	0.126717	1.844671	0.281436
13	6	0	-1.226893	1.567692	0.019789
14	6	0	0.726978	3.017561	-0.178289
15	6	0	-1.974070	2.520921	-0.686524
16	6	0	-0.033330	3.946889	-0.888271
17	1	0	1.775583	3.198072	0.034515
18	6	0	-1.386629	3.703916	-1.135615
19	1	0	-3.020597	2.320518	-0.895700
20	1	0	0.430978	4.863072	-1.239643
21	1	0	-1.980259	4.428272	-1.684266
22	6	0	-2.965725	0.381776	1.342145
23	6	0	-1.870452	-0.787565	-0.464061
24	6	0	-3.369984	-1.086176	1.450728
25	1	0	-2.700774	0.833012	2.303527
26	1	0	-3.783979	0.976581	0.905357
27	6	0	-3.083652	-1.613594	0.034700
28	1	0	-2.027198	-0.458454	-1.500821
29	1	0	-4.415527	-1.213154	1.740900
30	1	0	-2.743812	-1.596615	2.187906
31	1	0	-2.911236	-2.691898	0.006216
32	1	0	-3.932784	-1.406735	-0.623185
33	6	0	0.648763	-0.792554	-1.286538
34	6	0	-0.499188	-1.615124	-0.535479
35	1	0	0.902489	-1.345857	-2.191439
36	6	0	-0.746464	-2.840237	-1.323306
37	7	0	-0.950089	-3.779484	-1.974531
38	6	0	-0.107484	-2.046570	0.818342
39	7	0	0.169386	-2.420023	1.881399
40	7	0	-1.781930	0.332308	0.468000
41	1	0	0.192717	0.141204	-1.619217

1411aab_biphenylO_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.969231	3.779616	-1.068833
2	6	0	-1.690515	2.842007	-0.327244
3	6	0	-1.033674	1.881152	0.449833
4	6	0	0.364775	1.900038	0.482810
5	6	0	1.101360	2.828491	-0.249667
6	6	0	0.426468	3.767472	-1.032151
7	1	0	-1.494423	4.516313	-1.668163
8	1	0	-2.776494	2.849650	-0.353473
9	1	0	2.184939	2.814746	-0.201570
10	1	0	0.994492	4.495930	-1.602665
11	6	0	-1.783612	0.851819	1.253888
12	6	0	-1.973168	-0.554772	0.558000
13	1	0	-2.784175	1.226850	1.482927
14	6	0	-2.691896	-0.366407	-0.718767
15	7	0	-3.267313	-0.193082	-1.711479
16	6	0	-2.864663	-1.324895	1.455916
17	7	0	-3.541555	-1.905668	2.198117

18	6	0	1.976295	0.194290	0.785245
19	6	0	3.272275	0.339240	1.271245
20	6	0	1.647721	-0.764565	-0.197321
21	6	0	4.303407	-0.447692	0.758114
22	1	0	3.454366	1.084769	2.038387
23	6	0	2.708234	-1.531877	-0.709177
24	6	0	4.015202	-1.371135	-0.245717
25	1	0	5.315867	-0.329856	1.130177
26	1	0	2.518259	-2.280879	-1.467972
27	1	0	4.803780	-1.989081	-0.663839
28	7	0	0.293937	-0.884194	-0.636174
29	6	0	-0.655828	-1.430993	0.359088
30	1	0	-1.277829	0.658395	2.201976
31	6	0	0.064978	-1.640858	-1.887197
32	1	0	0.912744	-1.532171	-2.562960
33	1	0	-0.805561	-1.214333	-2.393189
34	6	0	-1.013800	-2.877895	-0.128526
35	1	0	-0.748597	-3.613701	0.633205
36	1	0	-2.088185	-2.979286	-0.307274
37	6	0	-0.230608	-3.079465	-1.441748
38	1	0	0.699112	-3.624464	-1.255049
39	1	0	-0.803074	-3.639714	-2.185313
40	1	0	-0.183014	-1.446987	1.341851
41	8	0	0.979998	0.990373	1.334119

1501aaa_model2_PhPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.957409	3.212738	0.769854
2	6	0	-2.126556	2.013303	0.091177
3	6	0	-1.016933	1.234212	-0.302309
4	6	0	0.299775	1.689393	0.008879
5	6	0	0.440228	2.905206	0.690495
6	6	0	-0.668080	3.660869	1.069545
7	1	0	-2.824070	3.800439	1.053583
8	1	0	-3.127989	1.695128	-0.170181
9	1	0	1.438358	3.252027	0.937511
10	1	0	-0.525427	4.597890	1.598903
11	6	0	-1.162662	0.015140	-1.074898
12	6	0	-2.243585	-0.811894	-1.228026
13	1	0	-0.276560	-0.291345	-1.621611
14	6	0	-3.500203	-0.683161	-0.554818
15	7	0	-4.532888	-0.622926	-0.020484
16	6	0	-2.141357	-1.946112	-2.098646
17	7	0	-2.065681	-2.869223	-2.803861
18	6	0	1.522407	0.947746	-0.418205
19	6	0	2.403875	1.623477	-1.278364
20	6	0	1.806868	-0.402798	-0.051247
21	6	0	3.512389	1.000053	-1.844953
22	1	0	2.176411	2.653747	-1.536753
23	6	0	2.911610	-1.030444	-0.671321
24	6	0	3.743835	-0.343933	-1.550233
25	1	0	4.163652	1.544728	-2.520578
26	1	0	3.135892	-2.064889	-0.444377
27	1	0	4.587465	-0.864987	-1.994073
28	7	0	1.018014	-1.100645	0.860749
29	6	0	1.215872	-2.543998	1.063940
30	1	0	2.255439	-2.778994	1.343181
31	1	0	0.983187	-3.097579	0.148059
32	6	0	0.284643	-2.871303	2.231091
33	1	0	0.560827	-3.802100	2.732640
34	1	0	-0.748522	-2.964786	1.878717
35	6	0	0.499897	-0.476279	2.103621
36	6	0	0.441799	-1.629224	3.118844
37	1	0	1.381787	-1.689776	3.678388
38	1	0	-0.370343	-1.500845	3.838968
39	1	0	1.153869	0.338237	2.431970
40	1	0	-0.498570	-0.055289	1.944250

1501aab_model2_PhPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.957660	-3.212451	0.770357
2	6	0	2.126816	-2.013103	0.091534
3	6	0	1.017182	-1.234135	-0.302191
4	6	0	-0.299533	-1.689376	0.008922
5	6	0	-0.439987	-2.905097	0.690684
6	6	0	0.668328	-3.660625	1.069970
7	1	0	2.824316	-3.800075	1.054260
8	1	0	3.128255	-1.694917	-0.169773
9	1	0	-1.438125	-3.251938	0.937648
10	1	0	0.525684	-4.597576	1.599454
11	6	0	1.162937	-0.015160	-1.074958
12	6	0	2.243792	0.811980	-1.228005
13	1	0	0.276909	0.291137	-1.621888
14	6	0	3.500258	0.683559	-0.554447
15	7	0	4.532965	0.623446	-0.020142
16	6	0	2.141595	1.946064	-2.098798
17	7	0	2.066078	2.869051	-2.804192
18	6	0	-1.522190	-0.947863	-0.418365
19	6	0	-2.403405	-1.623768	-1.278643
20	6	0	-1.806989	0.402596	-0.051384
21	6	0	-3.511982	-1.000583	-1.845357
22	1	0	-2.175676	-2.653988	-1.536998
23	6	0	-2.911856	1.029982	-0.671527
24	6	0	-3.743808	0.343328	-1.550572
25	1	0	-4.163012	-1.545384	-2.521106
26	1	0	-3.136463	2.064336	-0.444480
27	1	0	-4.587540	0.864194	-1.994436
28	7	0	-1.018411	1.100675	0.860686
29	6	0	-1.217040	2.543887	1.064088
30	1	0	-2.256656	2.778285	1.343701
31	1	0	-0.984964	3.097640	0.148167
32	6	0	-0.285565	2.871581	2.230900
33	1	0	-0.561948	3.802254	2.732553
34	1	0	0.747447	2.965494	1.878164
35	6	0	-0.500215	0.476401	2.103570
36	6	0	-0.441915	1.629447	3.118705
37	1	0	-1.381648	1.689749	3.678711
38	1	0	0.370601	1.501311	3.838435
39	1	0	-1.154268	-0.337984	2.432103
40	1	0	0.498162	0.055279	1.944108

1504aaa_model2_PhPh_pyrrolidine_CN2_TS_b3lyp631dp_PCMdmso_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.259538	3.323872	-0.320504
2	6	0	-1.656530	1.991812	-0.407630
3	6	0	-0.723046	0.949628	-0.530378
4	6	0	0.659869	1.279391	-0.559031
5	6	0	1.038152	2.629925	-0.488853
6	6	0	0.095497	3.648036	-0.363846
7	1	0	-2.009663	4.103234	-0.230033
8	1	0	-2.714220	1.762724	-0.400060
9	1	0	2.095060	2.875841	-0.519785
10	1	0	0.419059	4.682334	-0.302073
11	6	0	-1.168690	-0.479226	-0.691190
12	6	0	-2.540554	-0.891812	-0.932590
13	1	0	-0.491314	-1.023629	-1.352095
14	6	0	-3.660702	-0.391619	-0.236367
15	7	0	-4.602095	0.010310	0.335250
16	6	0	-2.770899	-2.019893	-1.750405
17	7	0	-2.957921	-2.947180	-2.442294
18	6	0	1.770050	0.280369	-0.691783
19	6	0	2.634594	0.329213	-1.796025
20	6	0	2.033591	-0.676070	0.307521
21	6	0	3.707641	-0.554909	-1.910114

22	1	0	2.451230	1.063643	-2.574176
23	6	0	3.105775	-1.563603	0.197945
24	6	0	3.945064	-1.503934	-0.914209
25	1	0	4.356994	-0.502544	-2.778308
26	1	0	3.276344	-2.286645	0.988974
27	1	0	4.780136	-2.191713	-0.998973
28	7	0	1.161493	-0.748732	1.440782
29	6	0	0.051479	-1.529367	1.418455
30	1	0	0.125651	-2.502547	0.931394
31	1	0	-0.777942	-0.999388	0.416931
32	6	0	-0.692760	-1.348565	2.721665
33	1	0	-1.775099	-1.434007	2.602712
34	1	0	-0.374222	-2.136590	3.415812
35	6	0	1.183145	0.197496	2.580622
36	1	0	1.971486	-0.112080	3.276934
37	1	0	1.403691	1.210883	2.239208
38	6	0	-0.225584	0.049399	3.184123
39	1	0	-0.219341	0.152602	4.270375
40	1	0	-0.887516	0.816229	2.772579

1505aaa_model2_PhPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.877542	-1.971306	2.416902
2	6	0	2.164702	-1.424425	1.168764
3	6	0	1.157093	-1.154808	0.230720
4	6	0	-0.178692	-1.432501	0.590207
5	6	0	-0.461097	-2.000235	1.845761
6	6	0	0.556147	-2.267686	2.758844
7	1	0	2.682092	-2.172306	3.118329
8	1	0	3.192793	-1.198607	0.901843
9	1	0	-1.492114	-2.228772	2.101608
10	1	0	0.318915	-2.702420	3.724938
11	6	0	1.539770	-0.649020	-1.160081
12	6	0	2.587596	0.455308	-1.213980
13	1	0	1.920567	-1.505529	-1.731403
14	6	0	2.216987	1.770970	-0.943352
15	7	0	1.861474	2.875056	-0.722995
16	6	0	3.918193	0.175635	-1.531502
17	7	0	5.035841	-0.078830	-1.807272
18	6	0	-1.321239	-1.190748	-0.350957
19	6	0	-1.809535	-2.242417	-1.139704
20	6	0	-1.950475	0.059184	-0.499753
21	6	0	-2.861635	-2.059122	-2.037279
22	1	0	-1.339960	-3.216382	-1.047739
23	6	0	-3.003254	0.258752	-1.396902
24	6	0	-3.457658	-0.805356	-2.172346
25	1	0	-3.212562	-2.896309	-2.631960
26	1	0	-3.471034	1.235225	-1.466161
27	1	0	-4.276191	-0.653617	-2.867617
28	7	0	-1.541760	1.193494	0.300056
29	6	0	-1.094062	2.309261	-0.173333
30	1	0	-0.894705	2.421988	-1.232467
31	1	0	0.635507	-0.332965	-1.689969
32	6	0	-0.935620	3.358388	0.862858
33	1	0	0.027375	3.858889	0.744528
34	1	0	-1.723048	4.109130	0.707631
35	6	0	-1.808664	1.272763	1.775312
36	1	0	-2.894912	1.306681	1.896536
37	1	0	-1.422640	0.376150	2.256394
38	6	0	-1.096224	2.571622	2.185269
39	1	0	-1.665600	3.122723	2.933610
40	1	0	-0.112615	2.342518	2.600694

1509aaa_model2_PhPh_pyrrolidine_CN2_PRODUCTb3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.896302	3.847245	-0.432833
2	6	0	-0.046725	3.043406	0.325101
3	6	0	-0.324397	1.687099	0.551035
4	6	0	-1.502412	1.131636	0.005111
5	6	0	-2.358683	1.957390	-0.742228
6	6	0	-2.062029	3.299956	-0.968407
7	1	0	-0.654098	4.893469	-0.592070
8	1	0	0.846957	3.478304	0.763907
9	1	0	-3.262889	1.527393	-1.162383
10	1	0	-2.738326	3.912742	-1.556686
11	6	0	0.610873	0.908284	1.454362
12	6	0	1.819475	0.171067	0.747544
13	1	0	1.042384	1.601225	2.180367
14	6	0	2.427946	1.042397	-0.274677
15	7	0	2.913678	1.723299	-1.079111
16	6	0	2.850857	-0.097419	1.770941
17	7	0	3.636175	-0.339789	2.590465
18	6	0	-1.899062	-0.286384	0.220823
19	6	0	-3.162511	-0.574106	0.767366
20	6	0	-1.058196	-1.358709	-0.139354
21	6	0	-3.585482	-1.886261	0.963829
22	1	0	-3.810420	0.250118	1.050097
23	6	0	-1.490839	-2.677372	0.067909
24	6	0	-2.743761	-2.944804	0.615093
25	1	0	-4.563669	-2.081525	1.392534
26	1	0	-0.836565	-3.499772	-0.206022
27	1	0	-3.059354	-3.972047	0.770491
28	7	0	0.221202	-1.092882	-0.733064
29	6	0	1.391978	-1.231069	0.129897
30	1	0	1.172678	-1.851311	1.008213
31	1	0	0.073274	0.143556	2.020842
32	6	0	2.479374	-1.885454	-0.752352
33	1	0	3.484289	-1.504001	-0.552208
34	1	0	2.492652	-2.959658	-0.545609
35	6	0	0.482660	-1.697059	-2.057053
36	1	0	0.139102	-2.740876	-2.104907
37	1	0	-0.045966	-1.137664	-2.835714
38	6	0	2.003728	-1.630465	-2.193002
39	1	0	2.388998	-2.370588	-2.898247
40	1	0	2.314629	-0.640024	-2.535269

1509aab_model2_PhPh_pyrrolidine_CN2_PRODUCTb3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.896706	3.847190	0.432729
2	6	0	0.047027	3.043396	-0.325135
3	6	0	0.324540	1.687034	-0.550986
4	6	0	1.502531	1.131502	-0.005087
5	6	0	2.358917	1.957211	0.742171
6	6	0	2.062398	3.299814	0.968295
7	1	0	0.654611	4.893446	0.591921
8	1	0	-0.846615	3.478363	-0.763952
9	1	0	3.263111	1.527148	1.162282
10	1	0	2.738788	3.912564	1.556503
11	6	0	-0.610808	0.908307	-1.454320
12	6	0	-1.819521	0.171186	-0.747556
13	1	0	-1.042264	1.601301	-2.180304
14	6	0	-2.428003	1.042572	0.274579
15	7	0	-2.913755	1.723476	1.079000
16	6	0	-2.850757	-0.097296	-1.771031
17	7	0	-3.635988	-0.339708	-2.590632
18	6	0	1.899054	-0.286555	-0.220785
19	6	0	3.162454	-0.574437	-0.767355
20	6	0	1.058073	-1.358770	0.139419
21	6	0	3.585245	-1.886651	-0.963821
22	1	0	3.810468	0.249698	-1.050104
23	6	0	1.490516	-2.677493	-0.067848
24	6	0	2.743394	-2.945086	-0.615066
25	1	0	4.563393	-2.082046	-1.392554
26	1	0	0.836141	-3.499802	0.206102

27	1	0	3.058851	-3.972369	-0.770473
28	7	0	-0.221287	-1.092713	0.733120
29	6	0	-1.392073	-1.230965	-0.129834
30	1	0	-1.172746	-1.851225	-1.008121
31	1	0	-0.073285	0.143538	-2.020816
32	6	0	-2.479469	-1.885278	0.752437
33	1	0	-3.484382	-1.503869	0.552248
34	1	0	-2.492720	-2.959504	0.545802
35	6	0	-0.482805	-1.696722	2.057197
36	1	0	-0.139196	-2.740504	2.105201
37	1	0	0.045740	-1.137177	2.835802
38	6	0	-2.003875	-1.630140	2.193071
39	1	0	-2.389174	-2.370182	2.898379
40	1	0	-2.314790	-0.639662	2.535226

1509aac_model2_PhPh_pyrrolidine_CN2_PRODUCTb3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.156305	-4.009930	0.426907
2	6	0	0.445405	-3.115214	-0.458272
3	6	0	-0.035053	-1.808775	-0.603150
4	6	0	-1.151830	-1.382559	0.151272
5	6	0	-1.742916	-2.295918	1.040447
6	6	0	-1.250740	-3.592901	1.184381
7	1	0	0.227352	-5.020877	0.522577
8	1	0	1.296717	-3.434789	-1.052656
9	1	0	-2.598459	-1.976963	1.627616
10	1	0	-1.725190	-4.274816	1.883631
11	6	0	0.673143	-0.836302	-1.507884
12	6	0	1.740801	0.009915	-0.709568
13	1	0	1.187324	-1.348406	-2.324269
14	6	0	2.917805	-0.838719	-0.433765
15	7	0	3.824803	-1.523872	-0.199968
16	6	0	2.172632	1.144058	-1.546877
17	7	0	2.487085	2.041147	-2.212558
18	6	0	-1.810053	-0.056289	-0.070716
19	6	0	-3.161418	-0.126696	-0.461323
20	6	0	-1.209984	1.233440	0.055145
21	6	0	-3.934807	0.993843	-0.742944
22	1	0	-3.602801	-1.114147	-0.556911
23	6	0	-2.003615	2.359874	-0.274884
24	6	0	-3.334650	2.248972	-0.655260
25	1	0	-4.972087	0.885391	-1.042258
26	1	0	-1.555027	3.344907	-0.244036
27	1	0	-3.894019	3.148875	-0.893969
28	7	0	0.088296	1.493827	0.512095
29	6	0	1.179358	0.542956	0.677410
30	1	0	0.862559	-0.347794	1.225201
31	1	0	-0.030633	-0.129597	-1.951564
32	6	0	2.257331	1.305840	1.482078
33	1	0	2.790814	0.638580	2.161446
34	1	0	2.994583	1.754006	0.807389
35	6	0	0.403591	2.780972	1.167097
36	1	0	0.778423	3.521046	0.446647
37	1	0	-0.494279	3.191172	1.634781
38	6	0	1.473650	2.410571	2.194128
39	1	0	2.100653	3.260680	2.473257
40	1	0	0.998709	2.022199	3.100821

1601aab_model3_PhPhPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.017666	3.542605	0.818846
2	6	0	-1.820675	2.420002	0.683232
3	6	0	-1.408679	1.318237	-0.099970
4	6	0	-0.141542	1.363582	-0.753477

5	6	0	0.646309	2.512685	-0.602871
6	6	0	0.219332	3.590690	0.168763
7	1	0	-1.348911	4.373833	1.432430
8	1	0	-2.762579	2.380500	1.215314
9	1	0	1.601550	2.563465	-1.112236
10	1	0	0.850306	4.469224	0.260977
11	6	0	-2.204543	0.110347	-0.201417
12	6	0	-3.539043	-0.097210	0.032654
13	1	0	-1.665101	-0.773991	-0.521874
14	6	0	-4.500283	0.908902	0.367414
15	7	0	-5.317877	1.695522	0.628712
16	6	0	-4.074871	-1.420488	-0.096333
17	7	0	-4.516156	-2.492842	-0.199000
18	6	0	2.475089	-0.071007	-0.327839
19	6	0	3.683236	0.582585	-0.611480
20	6	0	2.139890	-0.351117	1.028383
21	6	0	4.532022	1.043892	0.393739
22	1	0	3.931619	0.768463	-1.652997
23	6	0	2.985984	0.164896	2.034681
24	6	0	4.155744	0.853613	1.722985
25	1	0	5.451435	1.562689	0.141877
26	1	0	2.739351	0.005101	3.076858
27	1	0	4.782723	1.223990	2.529332
28	7	0	1.006414	-1.098434	1.361944
29	6	0	0.584250	-1.204014	2.765506
30	1	0	0.282293	-0.224121	3.150039
31	1	0	1.390688	-1.584812	3.413953
32	6	0	-0.553946	-2.221746	2.717355
33	1	0	-1.473064	-1.747075	2.357245
34	1	0	-0.759181	-2.662722	3.696116
35	6	0	0.693235	-2.363542	0.648557
36	6	0	0.330522	0.278690	-1.665769
37	6	0	-0.449419	-0.039525	-2.791743
38	6	0	1.574258	-0.378429	-1.483039
39	6	0	-0.022254	-0.973994	-3.734003
40	1	0	-1.389848	0.481612	-2.944661
41	6	0	1.992134	-1.303978	-2.450875
42	6	0	1.209497	-1.604672	-3.565555
43	1	0	-0.642884	-1.194919	-4.596752
44	1	0	2.944401	-1.806506	-2.310189
45	1	0	1.560420	-2.329394	-4.293933
46	6	0	-0.027486	-3.237087	1.692487
47	1	0	0.686596	-3.912509	2.175878
48	1	0	-0.813710	-3.849470	1.243555
49	1	0	1.608226	-2.837936	0.275494
50	1	0	0.052436	-2.178651	-0.219386

1601aac_model3_PhPhPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.235779	-2.818638	-1.763633
2	6	0	2.988641	-1.915239	-1.028571
3	6	0	2.420410	-0.714892	-0.545730
4	6	0	1.048331	-0.433651	-0.818170
5	6	0	0.312582	-1.366369	-1.560796
6	6	0	0.891837	-2.540990	-2.032910
7	1	0	2.688191	-3.739417	-2.116512
8	1	0	4.017097	-2.157382	-0.791828
9	1	0	-0.727352	-1.158475	-1.783706
10	1	0	0.296039	-3.239376	-2.612256
11	6	0	3.172207	0.197269	0.297773
12	6	0	4.525440	0.374266	0.414330
13	1	0	2.577934	0.842037	0.937431
14	6	0	5.523543	-0.266191	-0.387579
15	7	0	6.366411	-0.753757	-1.025650
16	6	0	5.032800	1.305579	1.378541
17	7	0	5.452295	2.060288	2.159184
18	6	0	-1.415526	-0.269855	0.985487
19	6	0	-0.615970	-1.062014	1.826358
20	6	0	-2.813809	-0.559416	0.892563
21	6	0	-1.128769	-2.095776	2.603737

22	1	0	0.440713	-0.823764	1.896761
23	6	0	-3.321326	-1.594098	1.718328
24	6	0	-2.500587	-2.343250	2.553170
25	1	0	-0.477067	-2.673200	3.251413
26	1	0	-4.378067	-1.825472	1.694310
27	1	0	-2.941027	-3.130046	3.159463
28	7	0	-3.688544	0.131144	0.059613
29	6	0	-5.134574	-0.135136	0.111664
30	1	0	-5.541709	0.116642	1.097144
31	1	0	-5.357039	-1.197362	-0.078295
32	6	0	-5.706921	0.724038	-1.016308
33	1	0	-5.823879	1.761541	-0.683781
34	1	0	-6.680867	0.363029	-1.356036
35	6	0	-3.319216	0.700079	-1.254235
36	6	0	0.416265	0.857857	-0.412511
37	6	0	1.006311	2.051466	-0.870109
38	6	0	-0.769453	0.927804	0.364009
39	6	0	0.463416	3.298073	-0.569739
40	1	0	1.893326	1.991704	-1.493457
41	6	0	-1.292373	2.198081	0.663117
42	6	0	-0.693421	3.369906	0.206353
43	1	0	0.938287	4.200588	-0.941359
44	1	0	-2.187080	2.256366	1.275052
45	1	0	-1.126331	4.332655	0.460767
46	6	0	-4.609384	0.622903	-2.082946
47	1	0	-4.675596	-0.343247	-2.595824
48	1	0	-4.658958	1.410576	-2.839236
49	1	0	-2.497626	0.138587	-1.709188
50	1	0	-2.987505	1.739454	-1.156039

1601aad_model3_PhPhPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.557938	0.363565	-0.561036
2	6	0	3.497585	1.120463	-0.083829
3	6	0	2.319842	0.507763	0.400019
4	6	0	2.218064	-0.912505	0.381270
5	6	0	3.312678	-1.652823	-0.085776
6	6	0	4.468325	-1.030851	-0.555144
7	1	0	5.456677	0.855905	-0.917059
8	1	0	3.599395	2.197359	-0.046004
9	1	0	3.244065	-2.735877	-0.093502
10	1	0	5.296866	-1.633611	-0.913623
11	6	0	1.253325	1.272454	1.014180
12	6	0	0.959213	2.608262	0.935279
13	1	0	0.592896	0.697652	1.656199
14	6	0	1.617856	3.564856	0.098407
15	7	0	2.114331	4.375016	-0.574221
16	6	0	-0.116340	3.143715	1.716885
17	7	0	-0.985306	3.591747	2.349046
18	6	0	-0.513365	-1.059057	-1.102241
19	6	0	0.415752	-1.251903	-2.140574
20	6	0	-1.740829	-0.382212	-1.405762
21	6	0	0.195611	-0.831535	-3.448091
22	1	0	1.326295	-1.794450	-1.915315
23	6	0	-1.955144	0.011589	-2.750503
24	6	0	-1.012629	-0.204100	-3.748036
25	1	0	0.939289	-1.016382	-4.216562
26	1	0	-2.876798	0.511621	-3.016712
27	1	0	-1.227542	0.126637	-4.760439
28	7	0	-2.740664	-0.124744	-0.469072
29	6	0	-4.043367	0.408715	-0.898736
30	1	0	-4.542547	-0.289761	-1.578878
31	1	0	-3.936543	1.369769	-1.427005
32	6	0	-4.797574	0.625097	0.412637
33	1	0	-5.213254	-0.322126	0.774129
34	1	0	-5.618040	1.338848	0.303914
35	6	0	-2.487297	0.232985	0.942418
36	6	0	1.024328	-1.678229	0.871897
37	6	0	1.221322	-2.449401	2.031941
38	6	0	-0.228529	-1.737294	0.202346

39	6	0	0.222214	-3.270642	2.546661
40	1	0	2.181766	-2.392154	2.535364
41	6	0	-1.212715	-2.594311	0.732135
42	6	0	-1.002457	-3.347896	1.883204
43	1	0	0.402865	-3.847915	3.448009
44	1	0	-2.162004	-2.668333	0.211542
45	1	0	-1.789454	-3.998075	2.253470
46	6	0	-3.680541	1.113694	1.343199
47	1	0	-3.458857	2.167477	1.143735
48	1	0	-3.921538	1.016884	2.404982
49	1	0	-1.534046	0.758744	1.041570
50	1	0	-2.437617	-0.658745	1.575432

1604aad_model3_PhPhPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso_TS_CH_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.533367	-1.666137	-3.524105
2	6	0	1.158350	-0.658699	-2.795365
3	6	0	1.020930	-0.569855	-1.399370
4	6	0	0.215384	-1.511740	-0.726616
5	6	0	-0.412738	-2.519212	-1.479024
6	6	0	-0.257702	-2.604963	-2.860064
7	1	0	0.659911	-1.713736	-4.601234
8	1	0	1.772820	0.074603	-3.310035
9	1	0	-1.032266	-3.244456	-0.960508
10	1	0	-0.754885	-3.395839	-3.413263
11	6	0	1.768197	0.559173	-0.727222
12	6	0	3.107010	0.333148	-0.232867
13	1	0	0.965053	0.979558	0.203235
14	6	0	3.970532	1.432659	-0.019085
15	7	0	4.675180	2.352092	0.153285
16	6	0	3.634296	-0.945709	0.046069
17	7	0	4.108676	-1.996868	0.250674
18	6	0	-2.235349	-0.268383	0.505392
19	6	0	-3.393424	-1.021723	0.263919
20	6	0	-2.179348	1.058095	-0.002092
21	6	0	-4.473761	-0.530014	-0.465151
22	1	0	-3.430088	-2.030911	0.662330
23	6	0	-3.278142	1.546053	-0.738461
24	6	0	-4.406346	0.765847	-0.969257
25	1	0	-5.347853	-1.150279	-0.633811
26	1	0	-3.264722	2.553365	-1.130666
27	1	0	-5.229943	1.182271	-1.540503
28	7	0	-1.091034	1.941171	0.203513
29	6	0	-1.081741	3.297133	-0.410645
30	1	0	-1.890807	3.887095	0.033384
31	1	0	-1.253664	3.230746	-1.487243
32	6	0	0.300704	3.866789	-0.065848
33	1	0	0.255235	4.937619	0.138228
34	1	0	0.992330	3.717076	-0.899273
35	6	0	0.036701	1.725123	0.948925
36	6	0	-0.016629	-1.514191	0.757859
37	6	0	0.888932	-2.180730	1.596634
38	6	0	-1.176427	-0.942352	1.327803
39	6	0	0.671121	-2.276790	2.971275
40	1	0	1.773097	-2.631867	1.161758
41	6	0	-1.393001	-1.062939	2.710201
42	6	0	-0.476384	-1.717628	3.531983
43	1	0	1.391707	-2.795251	3.596450
44	1	0	-2.290086	-0.626498	3.138929
45	1	0	-0.661987	-1.792395	4.599085
46	6	0	0.743552	3.045707	1.156107
47	1	0	1.825785	2.936227	1.249097
48	1	0	0.374487	3.485877	2.091214
49	1	0	1.713566	1.475307	-1.320447
50	1	0	-0.025935	1.014738	1.764996

1605aad_model3_PhPhPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.303971	-1.753289	-0.415623
2	6	0	3.447572	-0.981343	-1.200644
3	6	0	2.303439	-0.367198	-0.671406
4	6	0	2.009783	-0.555639	0.697781
5	6	0	2.887653	-1.323420	1.482440
6	6	0	4.024448	-1.922185	0.939209
7	1	0	5.181990	-2.213459	-0.859399
8	1	0	3.670893	-0.840247	-2.255135
9	1	0	2.661931	-1.459389	2.536472
10	1	0	4.679630	-2.514861	1.570532
11	6	0	1.474804	0.520071	-1.585498
12	6	0	1.708731	2.019580	-1.391343
13	1	0	0.410838	0.317481	-1.437536
14	6	0	2.969809	2.571749	-1.626120
15	7	0	4.043394	3.011382	-1.832661
16	6	0	0.658961	2.847982	-1.008174
17	7	0	-0.266980	3.508525	-0.688085
18	6	0	-0.928389	-1.445567	0.346532
19	6	0	-0.249455	-2.675757	0.332272
20	6	0	-2.032555	-1.328729	-0.532449
21	6	0	-0.621758	-3.722725	-0.507126
22	1	0	0.581265	-2.811319	1.013185
23	6	0	-2.413429	-2.376670	-1.376971
24	6	0	-1.704143	-3.573033	-1.372575
25	1	0	-0.069621	-4.656317	-0.476671
26	1	0	-3.252326	-2.250651	-2.051154
27	1	0	-2.001879	-4.377809	-2.035726
28	7	0	-2.851638	-0.138338	-0.587988
29	6	0	-4.352302	-0.231625	-0.603017
30	1	0	-4.664979	-0.958298	0.146864
31	1	0	-4.655748	-0.586227	-1.590486
32	6	0	-4.796439	1.213400	-0.324338
33	1	0	-5.043712	1.332833	0.732471
34	1	0	-5.672253	1.483749	-0.913883
35	6	0	-2.446136	1.087123	-0.644593
36	6	0	0.840878	0.059899	1.417136
37	6	0	1.137733	1.063729	2.355574
38	6	0	-0.504466	-0.376422	1.303531
39	6	0	0.161121	1.626056	3.173144
40	1	0	2.165882	1.401903	2.437525
41	6	0	-1.472016	0.176077	2.164414
42	6	0	-1.152999	1.166907	3.087856
43	1	0	0.429047	2.402898	3.882526
44	1	0	-2.488513	-0.203064	2.128166
45	1	0	-1.923200	1.566993	3.739627
46	6	0	-3.557252	2.067517	-0.676529
47	1	0	-3.597226	2.499826	-1.686050
48	1	0	-3.362237	2.898485	0.006606
49	1	0	1.687942	0.226204	-2.622121
50	1	0	-1.396531	1.351354	-0.685590

1609aaa_model3_PhPhPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.187233	-1.520490	1.292338
2	6	0	2.827993	-1.813363	1.357097
3	6	0	1.849550	-1.012026	0.744446
4	6	0	2.265596	0.126810	0.001727
5	6	0	3.646306	0.415844	-0.024373
6	6	0	4.597340	-0.378382	0.609669
7	1	0	4.908226	-2.166330	1.783742
8	1	0	2.503282	-2.687309	1.914944
9	1	0	3.974896	1.300239	-0.560306
10	1	0	5.647035	-0.104601	0.564479
11	6	0	0.413394	-1.358386	1.082311
12	6	0	-0.594632	-1.952851	0.012658
13	1	0	-0.058260	-0.471277	1.489057

14	6	0	-0.671041	-3.416309	0.210751
15	7	0	-0.748949	-4.558991	0.400733
16	6	0	-0.207212	-1.754731	-1.394467
17	7	0	0.051890	-1.681304	-2.523075
18	6	0	-0.401448	1.765181	0.794080
19	6	0	0.077913	2.584830	1.823726
20	6	0	-1.589276	1.029023	1.002347
21	6	0	-0.610165	2.692739	3.033895
22	1	0	0.993009	3.148337	1.667671
23	6	0	-2.284818	1.159752	2.211119
24	6	0	-1.799751	1.988027	3.224176
25	1	0	-0.222313	3.332582	3.820654
26	1	0	-3.200331	0.594580	2.362554
27	1	0	-2.345135	2.076313	4.158898
28	7	0	-2.025604	0.113947	-0.017742
29	6	0	-3.230002	0.481696	-0.783562
30	1	0	-3.023395	1.357676	-1.405688
31	1	0	-4.077021	0.728052	-0.122422
32	6	0	-3.520312	-0.779245	-1.594444
33	1	0	-2.866529	-0.819938	-2.470231
34	1	0	-4.556565	-0.829248	-1.936869
35	6	0	-2.038419	-1.320823	0.277726
36	6	0	1.424897	1.007769	-0.889154
37	6	0	1.913735	1.139967	-2.208592
38	6	0	0.265465	1.741907	-0.547384
39	6	0	1.312275	1.959577	-3.155911
40	1	0	2.784443	0.559738	-2.494786
41	6	0	-0.326408	2.575105	-1.516027
42	6	0	0.179472	2.693460	-2.805589
43	1	0	1.725442	2.021070	-4.158132
44	1	0	-1.199951	3.153058	-1.229558
45	1	0	-0.304031	3.349002	-3.523466
46	6	0	-3.171459	-1.902654	-0.602336
47	1	0	-4.030644	-2.121542	0.038139
48	1	0	-2.891047	-2.837018	-1.095055
49	1	0	0.426088	-2.080575	1.900526
50	1	0	-2.225922	-1.532934	1.339072

1611aab_model2_PhPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.072711	-0.731243	3.704543
2	6	0	-1.679950	-1.074085	2.494685
3	6	0	-0.912166	-1.338150	1.354593
4	6	0	0.496772	-1.290577	1.446250
5	6	0	1.095222	-0.950073	2.662995
6	6	0	0.317721	-0.662909	3.787457
7	1	0	-1.684661	-0.527700	4.578100
8	1	0	-2.763042	-1.137390	2.436942
9	1	0	2.178654	-0.916769	2.729007
10	1	0	0.798356	-0.402651	4.725779
11	6	0	-1.579731	-1.703476	0.045152
12	6	0	-2.107493	-0.505991	-0.845097
13	1	0	-2.440690	-2.352013	0.230390
14	6	0	-3.377348	-0.012909	-0.264772
15	7	0	-4.397492	0.309453	0.185717
16	6	0	-2.473604	-1.088060	-2.156059
17	7	0	-2.725523	-1.559324	-3.186154
18	6	0	1.990954	0.772162	-0.311870
19	6	0	3.303568	1.285534	-0.322378
20	6	0	0.917524	1.673854	-0.064467
21	6	0	3.598938	2.624986	-0.095496
22	1	0	4.116875	0.586712	-0.489991
23	6	0	1.236559	3.034919	0.128421
24	6	0	2.545016	3.506760	0.126105
25	1	0	4.628776	2.967363	-0.094423
26	1	0	0.443704	3.757889	0.265167
27	1	0	2.728788	4.565325	0.284414
28	7	0	-0.441194	1.244376	0.029623
29	6	0	-1.063922	0.665480	-1.164444
30	1	0	-0.891568	-2.265841	-0.584419

31	6	0	1.321002	-1.654378	0.252798
32	6	0	1.473966	-3.020548	-0.040753
33	6	0	1.901877	-0.696186	-0.605956
34	6	0	2.155501	-3.456348	-1.174627
35	1	0	1.039478	-3.747947	0.639209
36	6	0	2.570789	-1.157384	-1.758750
37	6	0	2.693607	-2.512984	-2.050052
38	1	0	2.256543	-4.518690	-1.374458
39	1	0	3.001643	-0.426083	-2.435495
40	1	0	3.211876	-2.827914	-2.950672
41	6	0	-1.437921	2.206117	0.541391
42	1	0	-0.988668	2.909527	1.238519
43	1	0	-2.178674	1.643877	1.114725
44	6	0	-1.768117	1.866077	-1.859333
45	1	0	-1.064636	2.311459	-2.566931
46	1	0	-2.652848	1.571835	-2.430640
47	6	0	-2.090111	2.855140	-0.705202
48	1	0	-1.658553	3.837848	-0.912055
49	1	0	-3.164560	2.991107	-0.564528
50	1	0	-0.302982	0.204149	-1.793762

1611aad_model2_PhPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.262542	-2.935975	1.950298
2	6	0	1.054140	-2.942205	1.258076
3	6	0	0.822013	-2.077443	0.176137
4	6	0	1.843722	-1.185132	-0.213196
5	6	0	3.063189	-1.201136	0.481116
6	6	0	3.276590	-2.063061	1.554905
7	1	0	2.414863	-3.617508	2.781476
8	1	0	0.275511	-3.641260	1.550341
9	1	0	3.852261	-0.524808	0.167510
10	1	0	4.229852	-2.055754	2.074684
11	6	0	-0.491750	-2.210524	-0.570508
12	6	0	-1.713944	-1.324021	-0.070897
13	1	0	-0.809199	-3.253574	-0.505516
14	6	0	-1.759606	-1.273246	1.400765
15	7	0	-1.805638	-1.244994	2.560013
16	6	0	-2.934496	-2.035082	-0.497732
17	7	0	-3.873480	-2.622651	-0.846750
18	6	0	0.977298	1.620005	0.244142
19	6	0	2.091252	2.155035	0.909188
20	6	0	-0.296499	1.689114	0.874972
21	6	0	2.001883	2.769479	2.155556
22	1	0	3.053030	2.100853	0.407222
23	6	0	-0.370497	2.320768	2.138230
24	6	0	0.750828	2.853718	2.764239
25	1	0	2.886720	3.179065	2.631963
26	1	0	-1.325074	2.382601	2.644829
27	1	0	0.639948	3.327245	3.735556
28	7	0	-1.491881	1.226970	0.306173
29	6	0	-1.660599	0.195815	-0.691144
30	1	0	-0.371871	-1.980372	-1.631660
31	6	0	1.675188	-0.232517	-1.357231
32	6	0	1.960803	-0.652980	-2.664390
33	6	0	1.225489	1.088659	-1.138024
34	6	0	1.799805	0.209438	-3.749429
35	1	0	2.312004	-1.667998	-2.826648
36	6	0	1.074631	1.946625	-2.238525
37	6	0	1.352955	1.513779	-3.535357
38	1	0	2.024839	-0.136042	-4.753839
39	1	0	0.735504	2.964092	-2.067699
40	1	0	1.227770	2.194703	-4.371832
41	6	0	-2.792642	1.788036	0.724693
42	1	0	-2.746406	2.882024	0.667540
43	1	0	-3.045777	1.520578	1.757094
44	6	0	-2.949390	0.634692	-1.402314
45	1	0	-2.672280	1.433531	-2.097241
46	1	0	-3.432693	-0.154500	-1.979001
47	6	0	-3.814326	1.189102	-0.261312

48	1	0	-4.534889	1.934074	-0.605236
49	1	0	-4.380817	0.383039	0.215332
50	1	0	-0.827781	0.169075	-1.384450

1701aaa_model3_NaphtPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.632333	-2.057760	-0.959051
2	6	0	-2.876833	-3.050349	-0.382643
3	6	0	-1.605541	-2.770104	0.187922
4	6	0	-1.090812	-1.426078	0.184605
5	6	0	-1.883185	-0.413637	-0.482050
6	6	0	-3.125684	-0.746756	-1.016802
7	1	0	-1.261899	-4.828424	0.748226
8	1	0	-4.598879	-2.279417	-1.398754
9	1	0	-3.240140	-4.073599	-0.355204
10	6	0	-0.851832	-3.823086	0.767949
11	6	0	0.155318	-1.177023	0.855051
12	1	0	-3.692943	0.006523	-1.550820
13	6	0	0.850547	-2.247170	1.403543
14	6	0	0.367766	-3.569500	1.348625
15	1	0	1.787809	-2.046514	1.913458
16	1	0	0.946670	-4.372725	1.793410
17	6	0	-1.367093	0.925906	-0.746291
18	6	0	-2.070753	2.099243	-0.755841
19	1	0	-0.320944	1.012135	-1.014606
20	6	0	-3.427021	2.236986	-0.315424
21	7	0	-4.521118	2.394873	0.049385
22	6	0	-1.432475	3.314122	-1.167487
23	7	0	-0.921323	4.304979	-1.501979
24	7	0	2.751222	0.004467	-0.252898
25	6	0	4.079770	0.517890	-0.621177
26	1	0	4.008222	1.520912	-1.070106
27	1	0	4.726795	0.596013	0.259667
28	6	0	4.594711	-0.490712	-1.650545
29	6	0	2.289383	-1.001203	-1.228861
30	1	0	1.269455	-0.792345	-1.563872
31	1	0	2.287574	-2.006577	-0.791052
32	6	0	3.308381	-0.910538	-2.372407
33	1	0	3.399747	-1.854379	-2.915928
34	1	0	3.008166	-0.135453	-3.086412
35	1	0	5.046393	-1.351521	-1.145125
36	1	0	5.345224	-0.054250	-2.314057
37	6	0	0.689328	0.197725	1.122596
38	6	0	-0.048750	0.981013	2.028398
39	6	0	1.952540	0.680597	0.653696
40	6	0	0.399844	2.208830	2.502077
41	1	0	-0.996765	0.584919	2.381896
42	6	0	2.401015	1.925005	1.170195
43	6	0	1.644998	2.667796	2.067978
44	1	0	-0.195435	2.779997	3.206694
45	1	0	3.356433	2.320488	0.851648
46	1	0	2.035319	3.616805	2.425049

1701aab_model3_NaphtPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.754482	-2.822329	-0.376992
2	6	0	3.607038	-1.748722	-0.285916
3	6	0	3.128928	-0.417038	-0.420898
4	6	0	1.729397	-0.168992	-0.646439
5	6	0	0.868876	-1.320660	-0.804499
6	6	0	1.391694	-2.602527	-0.649406
7	1	0	5.092831	0.447577	-0.166278
8	1	0	3.125265	-3.836899	-0.277746
9	1	0	4.668153	-1.900525	-0.110562

10	6	0	4.041524	0.666133	-0.328458
11	6	0	1.280391	1.195659	-0.666267
12	1	0	0.748792	-3.460007	-0.811763
13	6	0	2.221109	2.214388	-0.595403
14	6	0	3.599010	1.961947	-0.441139
15	1	0	1.871414	3.241655	-0.625414
16	1	0	4.295441	2.792303	-0.381324
17	6	0	-0.506979	-1.213984	-1.284301
18	6	0	-1.570342	-1.968169	-0.872885
19	1	0	-0.705629	-0.509625	-2.084057
20	6	0	-1.542601	-2.847257	0.258598
21	7	0	-1.568933	-3.551126	1.185588
22	6	0	-2.835908	-1.857141	-1.535406
23	7	0	-3.867571	-1.778194	-2.068449
24	7	0	-0.842178	0.834314	1.465064
25	6	0	-1.917518	0.478053	2.402360
26	1	0	-2.539083	1.349928	2.664585
27	1	0	-2.575908	-0.280037	1.965681
28	6	0	-1.164077	-0.014125	3.637298
29	6	0	0.408846	1.124490	2.207089
30	1	0	0.768220	2.135068	1.989279
31	1	0	1.201575	0.423636	1.927462
32	6	0	0.027973	0.950567	3.687114
33	1	0	0.865177	0.580606	4.284568
34	1	0	-0.289266	1.909563	4.111475
35	1	0	-0.822710	-1.043901	3.483967
36	1	0	-1.782257	0.011571	4.538168
37	6	0	-0.158985	1.590812	-0.793915
38	6	0	-0.540662	2.203100	-1.999536
39	6	0	-1.141632	1.384435	0.224389
40	6	0	-1.859451	2.554876	-2.275508
41	1	0	0.227659	2.365987	-2.750145
42	6	0	-2.480509	1.723586	-0.088978
43	6	0	-2.831649	2.288709	-1.310334
44	1	0	-2.121835	3.009558	-3.225116
45	1	0	-3.257839	1.558125	0.645886
46	1	0	-3.872932	2.535609	-1.497505

1704aab_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso_TS_CH_f2.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.598853	-1.885241	-0.048382
2	6	0	3.912825	-0.654684	0.464393
3	6	0	2.903973	0.308724	0.731361
4	6	0	1.501307	0.028332	0.479913
5	6	0	1.209998	-1.300939	-0.024318
6	6	0	2.247888	-2.186054	-0.291581
7	1	0	4.393568	1.706832	1.423623
8	1	0	4.367608	-2.620365	-0.262225
9	1	0	4.944262	-0.385583	0.672046
10	6	0	3.331571	1.557735	1.252836
11	6	0	0.572776	1.110568	0.759660
12	1	0	1.999605	-3.165610	-0.688462
13	6	0	1.065896	2.307652	1.274030
14	6	0	2.427664	2.547075	1.530106
15	1	0	0.357249	3.104395	1.473092
16	1	0	2.743694	3.505240	1.929460
17	6	0	-0.143584	-1.881744	-0.325957
18	6	0	-1.086853	-2.160178	0.741808
19	1	0	-0.052818	-2.735159	-1.002346
20	6	0	-0.900672	-1.735953	2.071605
21	7	0	-0.735465	-1.437296	3.192913
22	6	0	-2.193668	-2.997425	0.484113
23	7	0	-3.110613	-3.688988	0.251375
24	7	0	-0.930355	0.959337	-1.857816
25	6	0	0.187424	1.707767	-2.470069
26	1	0	-0.230259	2.490666	-3.114005
27	1	0	0.801108	2.186748	-1.704744
28	6	0	0.942763	0.628442	-3.270321
29	6	0	-1.031524	-0.319031	-2.308296
30	1	0	-2.021229	-0.779224	-2.293991

31	6	0	-0.095779	-0.497900	-3.479916
32	1	0	0.344864	-1.497281	-3.515218
33	1	0	-0.667509	-0.361815	-4.406305
34	1	0	1.784634	0.253213	-2.683146
35	1	0	1.333327	1.016582	-4.212385
36	6	0	-0.927903	1.179063	0.595947
37	6	0	-1.698124	1.386376	1.754493
38	6	0	-1.601630	1.285808	-0.638973
39	6	0	-3.061396	1.669938	1.697646
40	1	0	-1.208322	1.300705	2.717696
41	6	0	-2.965950	1.584245	-0.702322
42	6	0	-3.701653	1.779814	0.463718
43	1	0	-3.617940	1.812302	2.618733
44	1	0	-3.436549	1.656113	-1.677628
45	1	0	-4.760230	2.011799	0.406668
46	1	0	-0.605251	-1.105273	-1.235136

1705aab_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.246763	3.317953	-1.143473
2	6	0	1.355695	3.774054	-0.203913
3	6	0	0.488329	2.874141	0.467155
4	6	0	0.532709	1.454359	0.182630
5	6	0	1.478456	1.008085	-0.811457
6	6	0	2.293130	1.941865	-1.433930
7	1	0	-0.423077	4.469966	1.599772
8	1	0	2.908081	4.004622	-1.662852
9	1	0	1.293562	4.830783	0.039789
10	6	0	-0.427102	3.398802	1.418848
11	6	0	-0.399274	0.623458	0.913349
12	1	0	3.003575	1.584877	-2.174558
13	6	0	-1.270364	1.193788	1.830031
14	6	0	-1.295964	2.578804	2.091013
15	1	0	-1.951140	0.544136	2.372166
16	1	0	-1.994803	2.978859	2.818497
17	6	0	1.695985	-0.436078	-1.241011
18	6	0	2.909308	-1.095428	-0.577049
19	1	0	1.861140	-0.430583	-2.325011
20	6	0	3.405905	-0.670605	0.654524
21	7	0	3.817455	-0.301480	1.697114
22	6	0	3.498997	-2.202876	-1.190022
23	7	0	3.981426	-3.130705	-1.734678
24	7	0	-2.564964	-0.768801	-0.563933
25	6	0	-4.034383	-1.044431	-0.431345
26	1	0	-4.249192	-1.972061	-0.966851
27	1	0	-4.269576	-1.177923	0.624359
28	6	0	-4.680853	0.188993	-1.082762
29	6	0	-2.326667	0.192751	-1.393693
30	1	0	-1.311072	0.477553	-1.640419
31	6	0	-3.559923	0.789944	-1.963133
32	1	0	-3.512897	1.882500	-1.952096
33	1	0	-3.628441	0.490975	-3.018317
34	1	0	-4.975401	0.906581	-0.314434
35	1	0	-5.565592	-0.079257	-1.659676
36	6	0	-0.508845	-0.873086	0.817681
37	6	0	0.378324	-1.682118	1.543715
38	6	0	-1.585471	-1.522263	0.174642
39	6	0	0.217427	-3.065261	1.610590
40	1	0	1.203118	-1.207702	2.063247
41	6	0	-1.758432	-2.907861	0.241717
42	6	0	-0.849118	-3.682007	0.956588
43	1	0	0.923262	-3.659630	2.181747
44	1	0	-2.587035	-3.379750	-0.273412
45	1	0	-0.979321	-4.757761	1.002327
46	1	0	0.789602	-1.029181	-1.087969

1705aac_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.851640	1.805456	0.066477
2	6	0	2.961373	2.848852	0.141144
3	6	0	1.579395	2.633216	-0.091089
4	6	0	1.084693	1.314162	-0.430586
5	6	0	2.030947	0.224914	-0.407193
6	6	0	3.370223	0.507820	-0.184210
7	1	0	1.105950	4.704283	0.292510
8	1	0	4.912863	1.967724	0.229258
9	1	0	3.296648	3.854489	0.378312
10	6	0	0.691934	3.738031	0.018234
11	6	0	-0.324767	1.223649	-0.750979
12	1	0	4.070679	-0.322128	-0.169005
13	6	0	-1.141839	2.337836	-0.626670
14	6	0	-0.650632	3.594776	-0.219403
15	1	0	-2.188968	2.250269	-0.900887
16	1	0	-1.327883	4.438500	-0.135480
17	6	0	1.686648	-1.265773	-0.537099
18	6	0	2.140322	-2.120076	0.646606
19	1	0	2.159036	-1.657810	-1.445306
20	6	0	1.441929	-2.010108	1.846460
21	7	0	0.796612	-1.865754	2.825138
22	6	0	3.243847	-2.968065	0.558942
23	7	0	4.175764	-3.684280	0.463433
24	7	0	-2.473557	-0.374727	0.573506
25	6	0	-3.907730	-0.049266	0.871329
26	1	0	-4.127660	0.905000	0.385152
27	1	0	-4.550247	-0.816188	0.440832
28	6	0	-3.943836	0.012820	2.407192
29	6	0	-1.717024	-0.241379	1.612597
30	1	0	-0.651645	-0.438523	1.574701
31	6	0	-2.463285	0.188768	2.819888
32	1	0	-2.161313	-0.393239	3.694336
33	1	0	-2.193353	1.233576	3.029008
34	1	0	-4.336091	-0.922114	2.812058
35	1	0	-4.574137	0.829159	2.759192
36	6	0	-0.983501	0.029019	-1.372270
37	6	0	-0.646921	-0.330921	-2.688692
38	6	0	-2.035127	-0.687751	-0.765514
39	6	0	-1.300730	-1.361544	-3.357031
40	1	0	0.143708	0.221049	-3.185986
41	6	0	-2.699010	-1.725354	-1.429406
42	6	0	-2.327077	-2.067482	-2.724741
43	1	0	-1.014002	-1.610006	-4.373679
44	1	0	-3.486428	-2.274662	-0.925621
45	1	0	-2.837267	-2.877047	-3.235016
46	1	0	0.619550	-1.408597	-0.682826

1705aad_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.167253	2.509230	0.658264
2	6	0	-3.795742	1.307115	0.444125
3	6	0	-3.105336	0.229757	-0.168673
4	6	0	-1.713974	0.365584	-0.547703
5	6	0	-1.109564	1.663294	-0.379445
6	6	0	-1.839030	2.675687	0.224531
7	1	0	-4.858877	-1.030216	-0.129255
8	1	0	-3.692715	3.335982	1.126372
9	1	0	-4.834046	1.161581	0.728337
10	6	0	-3.814068	-0.976487	-0.422020
11	6	0	-1.078254	-0.815305	-1.091205
12	1	0	-1.360435	3.643390	0.347816
13	6	0	-1.832582	-1.948367	-1.356417
14	6	0	-3.203488	-2.038234	-1.037863
15	1	0	-1.335349	-2.811437	-1.788947
16	1	0	-3.750469	-2.950124	-1.254751
17	6	0	0.264464	2.064978	-0.902315

18	6	0	1.266865	2.448349	0.186610
19	1	0	0.121572	2.936047	-1.553773
20	6	0	1.217139	1.864488	1.436666
21	7	0	1.142447	1.331631	2.492155
22	6	0	2.333277	3.302766	-0.122102
23	7	0	3.211656	4.030880	-0.408232
24	7	0	1.061759	-1.468822	0.961696
25	6	0	-0.097521	-2.277888	1.462163
26	1	0	-0.982032	-1.639270	1.480122
27	1	0	-0.271872	-3.108455	0.779843
28	6	0	0.360775	-2.699262	2.865740
29	6	0	1.811972	-1.053815	1.948213
30	1	0	2.709927	-0.486146	1.758400
31	6	0	1.398102	-1.624793	3.263072
32	1	0	2.263836	-2.024867	3.799149
33	1	0	0.976016	-0.823065	3.874679
34	1	0	0.834327	-3.683168	2.824171
35	1	0	-0.477421	-2.752341	3.561425
36	6	0	0.385253	-0.968110	-1.396673
37	6	0	0.794559	-0.924536	-2.741965
38	6	0	1.368991	-1.281116	-0.433224
39	6	0	2.118125	-1.123945	-3.121034
40	1	0	0.043684	-0.706444	-3.494494
41	6	0	2.702995	-1.494970	-0.815511
42	6	0	3.081496	-1.400725	-2.148729
43	1	0	2.394233	-1.072628	-4.169165
44	1	0	3.434132	-1.777702	-0.066018
45	1	0	4.115656	-1.573914	-2.426758
46	1	0	0.675596	1.284788	-1.543505

1705aae_model3_NaphtPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.526887	-3.537403	-1.444876
2	6	0	-1.038937	-3.615437	-0.175238
3	6	0	-0.882790	-2.533533	0.732945
4	6	0	-0.207413	-1.324651	0.322413
5	6	0	0.413028	-1.313005	-0.981923
6	6	0	0.214058	-2.396955	-1.821872
7	1	0	-1.880009	-3.595983	2.326988
8	1	0	-0.651125	-4.356880	-2.146087
9	1	0	-1.567342	-4.502823	0.161389
10	6	0	-1.389944	-2.665759	2.053670
11	6	0	-0.198282	-0.237177	1.270380
12	1	0	0.681821	-2.380995	-2.802363
13	6	0	-0.674989	-0.432656	2.559354
14	6	0	-1.254289	-1.651021	2.968263
15	1	0	-0.646615	0.399903	3.255638
16	1	0	-1.623082	-1.760774	3.982979
17	6	0	1.404478	-0.265058	-1.469367
18	6	0	2.778466	-0.375801	-0.798526
19	1	0	1.040310	0.752388	-1.315834
20	6	0	3.274037	-1.593947	-0.329363
21	7	0	3.690390	-2.618233	0.080715
22	6	0	3.640503	0.722136	-0.822265
23	7	0	4.348387	1.664990	-0.850916
24	7	0	-1.788091	1.508144	-0.498653
25	6	0	-3.009267	1.102064	0.275181
26	1	0	-2.797538	0.145953	0.754667
27	1	0	-3.189309	1.853563	1.044332
28	6	0	-4.100790	1.022603	-0.808377
29	6	0	-1.966823	1.428494	-1.773730
30	1	0	-1.162194	1.674365	-2.458731
31	6	0	-3.324077	0.961173	-2.146620
32	1	0	-3.748006	1.578960	-2.943284
33	1	0	-3.233929	-0.055128	-2.553608
34	1	0	-4.724747	1.917771	-0.780704
35	1	0	-4.742750	0.153918	-0.663936
36	6	0	0.194668	1.172014	0.956285
37	6	0	1.318052	1.750314	1.561083
38	6	0	-0.581978	2.006003	0.130059

39	6	0	1.662685	3.084009	1.339925
40	1	0	1.935328	1.128588	2.199633
41	6	0	-0.248806	3.342190	-0.104602
42	6	0	0.883624	3.881559	0.502013
43	1	0	2.543469	3.496834	1.820247
44	1	0	-0.886633	3.953190	-0.734317
45	1	0	1.144804	4.919379	0.325680
46	1	0	1.482799	-0.387472	-2.559573

1709aab_model3_NaphtPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.806087	-1.512689	-1.153364
2	6	0	4.170165	-0.646396	-0.152968
3	6	0	3.233170	0.271451	0.392456
4	6	0	1.886565	0.329198	-0.121725
5	6	0	1.508284	-0.664400	-1.094268
6	6	0	2.467424	-1.530097	-1.595599
7	1	0	4.652361	1.045491	1.826958
8	1	0	4.524996	-2.204927	-1.579709
9	1	0	5.182138	-0.647836	0.242074
10	6	0	3.635977	1.127734	1.452561
11	6	0	1.020965	1.364823	0.391011
12	1	0	2.170901	-2.265450	-2.337945
13	6	0	1.466330	2.159176	1.436984
14	6	0	2.757606	2.032088	1.992978
15	1	0	0.804984	2.933427	1.813309
16	1	0	3.056710	2.676998	2.813296
17	6	0	0.080834	-0.912400	-1.533831
18	6	0	-0.767077	-1.729832	-0.468355
19	1	0	0.089974	-1.505421	-2.451195
20	6	0	-0.098519	-3.019374	-0.209817
21	7	0	0.436075	-4.025421	0.012630
22	6	0	-2.080485	-2.019065	-1.075376
23	7	0	-3.105535	-2.221727	-1.580722
24	7	0	-1.832069	0.205762	0.789559
25	6	0	-3.187152	-0.085081	1.298892
26	1	0	-3.481733	0.698775	2.007003
27	1	0	-3.930567	-0.099642	0.494333
28	6	0	-3.085961	-1.472717	1.957735
29	6	0	-0.945870	-0.935030	0.916418
30	1	0	0.063611	-0.635944	1.189664
31	6	0	-1.577211	-1.748714	2.059262
32	1	0	-1.328101	-2.810835	2.018575
33	1	0	-1.178607	-1.355756	2.999085
34	1	0	-3.575770	-2.223739	1.333624
35	1	0	-3.571174	-1.493435	2.935804
36	6	0	-0.264719	1.833979	-0.245741
37	6	0	-0.122813	2.958849	-1.073617
38	6	0	-1.577037	1.356488	0.035250
39	6	0	-1.210785	3.654062	-1.598352
40	1	0	0.884694	3.305078	-1.284957
41	6	0	-2.670449	2.098648	-0.466024
42	6	0	-2.492508	3.224790	-1.264142
43	1	0	-1.055248	4.522219	-2.230451
44	1	0	-3.680097	1.781733	-0.241617
45	1	0	-3.366494	3.755126	-1.631196
46	1	0	-0.468808	0.000885	-1.749134

1709aac_model3_NaphtPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.806129	-1.512733	-1.153260
2	6	0	4.170198	-0.646379	-0.152914
3	6	0	3.233200	0.271496	0.392457
4	6	0	1.886593	0.329205	-0.121731

5	6	0	1.508330	-0.664441	-1.094238
6	6	0	2.467472	-1.530162	-1.595515
7	1	0	4.652379	1.045644	1.826913
8	1	0	4.525041	-2.205004	-1.579544
9	1	0	5.182173	-0.647788	0.242122
10	6	0	3.635992	1.127839	1.452514
11	6	0	1.020974	1.364828	0.390955
12	1	0	2.170958	-2.265544	-2.337836
13	6	0	1.466320	2.159230	1.436902
14	6	0	2.757599	2.032200	1.992892
15	1	0	0.804958	2.933473	1.813213
16	1	0	3.056696	2.677161	2.813171
17	6	0	0.080888	-0.912417	-1.533841
18	6	0	-0.767100	-1.729820	-0.468375
19	1	0	0.090035	-1.505458	-2.451191
20	6	0	-0.098644	-3.019420	-0.209914
21	7	0	0.435831	-4.025541	0.012478
22	6	0	-2.080547	-2.018861	-1.075383
23	7	0	-3.105592	-2.221327	-1.580813
24	7	0	-1.831999	0.205750	0.789665
25	6	0	-3.187084	-0.085152	1.298970
26	1	0	-3.481682	0.698666	2.007114
27	1	0	-3.930470	-0.099675	0.494384
28	6	0	-3.085859	-1.472818	1.957751
29	6	0	-0.945814	-0.935056	0.916446
30	1	0	0.063685	-0.635982	1.189628
31	6	0	-1.577101	-1.748762	2.059284
32	1	0	-1.327952	-2.810874	2.018625
33	1	0	-1.178514	-1.355772	2.999103
34	1	0	-3.575635	-2.223835	1.333598
35	1	0	-3.571084	-1.493615	2.935813
36	6	0	-0.264724	1.833933	-0.245807
37	6	0	-0.122873	2.958753	-1.073754
38	6	0	-1.577022	1.356456	0.035316
39	6	0	-1.210884	3.653956	-1.598423
40	1	0	0.884621	3.304962	-1.285195
41	6	0	-2.670472	2.098649	-0.465837
42	6	0	-2.492583	3.224744	-1.264032
43	1	0	-1.055402	4.522068	-2.230598
44	1	0	-3.680105	1.781814	-0.241245
45	1	0	-3.366592	3.755104	-1.630997
46	1	0	-0.468719	0.000884	-1.749165

1709aad_model3_NaphtPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.671884	-1.843841	-0.938174
2	6	0	4.084017	-0.905959	-0.026565
3	6	0	3.216150	0.140739	0.385501
4	6	0	1.878536	0.245909	-0.153986
5	6	0	1.444712	-0.817278	-1.028683
6	6	0	2.346297	-1.797667	-1.413649
7	1	0	4.699683	0.959525	1.724501
8	1	0	4.339752	-2.632169	-1.270440
9	1	0	5.085767	-0.939704	0.392350
10	6	0	3.695662	1.086972	1.329861
11	6	0	1.115195	1.413208	0.216237
12	1	0	2.006734	-2.581965	-2.084606
13	6	0	1.639283	2.304487	1.142188
14	6	0	2.910887	2.138774	1.727425
15	1	0	1.050574	3.178027	1.404918
16	1	0	3.269620	2.860273	2.454789
17	6	0	0.016471	-1.041051	-1.485764
18	6	0	-0.891207	-1.832058	-0.427973
19	1	0	0.045035	-1.642602	-2.395158
20	6	0	-0.095225	-2.339874	0.708151
21	7	0	0.481208	-2.753925	1.626169
22	6	0	-1.489484	-3.003855	-1.100873
23	7	0	-1.982838	-3.898888	-1.651245
24	7	0	-1.546226	0.267533	0.779404
25	6	0	-2.241024	0.466173	2.080759

26	1	0	-1.569379	0.187006	2.902264
27	1	0	-2.504184	1.518993	2.210415
28	6	0	-3.462809	-0.460961	2.036101
29	6	0	-2.071767	-0.936899	0.126914
30	1	0	-2.667791	-0.682440	-0.760373
31	6	0	-2.962706	-1.630509	1.177434
32	1	0	-3.765100	-2.204747	0.709498
33	1	0	-2.371051	-2.316984	1.792137
34	1	0	-4.303992	0.039987	1.544347
35	1	0	-3.793553	-0.776550	3.029021
36	6	0	-0.156815	1.891137	-0.428138
37	6	0	-0.065031	2.967603	-1.327892
38	6	0	-1.432725	1.413008	-0.081371
39	6	0	-1.203672	3.563926	-1.867476
40	1	0	0.918338	3.340377	-1.597789
41	6	0	-2.575177	2.028637	-0.615467
42	6	0	-2.467611	3.099537	-1.500674
43	1	0	-1.103075	4.391950	-2.562491
44	1	0	-3.556887	1.656671	-0.335933
45	1	0	-3.363119	3.562458	-1.903995
46	1	0	-0.505431	-0.122091	-1.737072

1801aaa_model4_PhOCH2Ph_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.774368	-2.672805	-0.497441
2	6	0	-3.740999	-1.315697	-0.219790
3	6	0	-2.544348	-0.570597	-0.324003
4	6	0	-1.354169	-1.258448	-0.726179
5	6	0	-1.397647	-2.630527	-1.005509
6	6	0	-2.599229	-3.324506	-0.889832
7	1	0	-4.705208	-3.222700	-0.414376
8	1	0	-4.655288	-0.816487	0.073257
9	1	0	-0.503760	-3.159702	-1.307959
10	1	0	-2.616119	-4.387669	-1.108984
11	6	0	-2.440319	0.843974	-0.073620
12	6	0	-3.355816	1.753513	0.396877
13	1	0	-1.465118	1.265661	-0.293031
14	6	0	-4.700990	1.475199	0.792693
15	7	0	-5.801009	1.290558	1.128313
16	6	0	-2.965934	3.125131	0.532358
17	7	0	-2.657308	4.242299	0.645743
18	6	0	2.084098	-0.078335	-1.358864
19	6	0	2.189983	0.608554	-2.576552
20	6	0	3.030849	0.182732	-0.321677
21	6	0	3.209788	1.517044	-2.841478
22	1	0	1.453291	0.392685	-3.346817
23	6	0	4.088845	1.076622	-0.628010
24	6	0	4.172648	1.727506	-1.853338
25	1	0	3.266523	2.024507	-3.798737
26	1	0	4.852200	1.275613	0.112467
27	1	0	4.999651	2.409799	-2.030393
28	7	0	2.991342	-0.422710	0.927858
29	6	0	4.084863	-0.213105	1.891764
30	1	0	4.250764	0.858178	2.085674
31	1	0	5.023862	-0.630422	1.511812
32	6	0	3.589737	-0.897403	3.166529
33	1	0	4.088772	-0.513567	4.059755
34	1	0	3.765982	-1.977622	3.114022
35	6	0	1.742862	-0.778798	1.642759
36	6	0	1.006471	-1.123913	-1.274903
37	6	0	2.085982	-0.597461	3.127510
38	1	0	1.491255	-1.252073	3.769795
39	1	0	1.902725	0.437922	3.436016
40	1	0	1.463054	-1.823180	1.455185
41	1	0	0.913583	-0.146460	1.316386
42	1	0	0.817810	-1.536615	-2.270644
43	1	0	1.278738	-1.946134	-0.610771
44	8	0	-0.228467	-0.514355	-0.802728

1804aaa_model4_PhOCH2Ph_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso_TS_CH_f2_FRQ.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.288961	-1.979750	-0.589628
2	6	0	-3.700680	-0.720594	-0.504379
3	6	0	-2.302546	-0.560398	-0.480836
4	6	0	-1.505952	-1.718260	-0.533484
5	6	0	-2.098740	-2.982782	-0.617854
6	6	0	-3.483409	-3.118510	-0.650594
7	1	0	-5.370487	-2.067163	-0.607792
8	1	0	-4.328599	0.163974	-0.458419
9	1	0	-1.446020	-3.848325	-0.663735
10	1	0	-3.929771	-4.105465	-0.720539
11	6	0	-1.825851	0.867813	-0.421702
12	6	0	-1.913165	1.601880	0.764711
13	1	0	-0.315449	0.811125	-0.865134
14	6	0	-1.798017	1.008235	2.052188
15	7	0	-1.691322	0.554742	3.121304
16	6	0	-2.049564	3.018675	0.742570
17	7	0	-2.174791	4.178880	0.725477
18	6	0	2.005152	-1.321284	0.474598
19	6	0	2.829739	-2.400991	0.813534
20	6	0	2.588949	-0.147071	-0.051726
21	6	0	4.214505	-2.332716	0.677580
22	1	0	2.369237	-3.301395	1.211095
23	6	0	3.987044	-0.083500	-0.182250
24	6	0	4.789943	-1.161949	0.180431
25	1	0	4.834706	-3.177439	0.959442
26	1	0	4.448918	0.809624	-0.587610
27	1	0	5.866864	-1.086863	0.063104
28	7	0	1.806206	0.971567	-0.422084
29	6	0	2.194662	2.343368	-0.033345
30	1	0	3.236390	2.545434	-0.305449
31	1	0	2.105414	2.468670	1.050742
32	6	0	1.232759	3.246427	-0.824398
33	1	0	1.744467	4.143069	-1.180815
34	1	0	0.394494	3.563578	-0.198788
35	6	0	0.758732	0.957355	-1.371406
36	6	0	0.525084	-1.426904	0.697555
37	6	0	0.747824	2.354386	-1.983466
38	1	0	-0.229626	2.639778	-2.380534
39	1	0	1.462693	2.384325	-2.813974
40	1	0	0.784853	0.104659	-2.050631
41	1	0	0.297998	-2.257013	1.376068
42	1	0	0.140368	-0.505846	1.145217
43	8	0	-0.127767	-1.666238	-0.572826
44	1	0	-2.070007	1.448262	-1.311095

1805aaa_model4_PhOCH2Ph_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.766668	-2.108303	1.565723
2	6	0	-3.655627	-1.338623	0.406604
3	6	0	-2.416308	-0.993249	-0.141352
4	6	0	-1.258123	-1.449818	0.521244
5	6	0	-1.353667	-2.217284	1.689688
6	6	0	-2.608831	-2.544799	2.207171
7	1	0	-4.745216	-2.362284	1.961623
8	1	0	-4.553689	-0.986315	-0.094335
9	1	0	-0.464437	-2.561220	2.203736
10	1	0	-2.670926	-3.141634	3.112334
11	6	0	-2.346230	-0.146742	-1.408514
12	6	0	-2.956641	1.249689	-1.285112
13	1	0	-1.305406	-0.076262	-1.733392
14	6	0	-2.268621	2.257012	-0.609459
15	7	0	-1.659981	3.094008	-0.041718
16	6	0	-4.242500	1.510794	-1.759464

17	7	0	-5.326925	1.713259	-2.177933
18	6	0	2.303157	-1.272085	-0.384787
19	6	0	2.774149	-2.173893	-1.345824
20	6	0	2.955106	-0.031865	-0.297554
21	6	0	3.845075	-1.855358	-2.181033
22	1	0	2.293214	-3.143443	-1.430683
23	6	0	4.025959	0.306070	-1.124036
24	6	0	4.474064	-0.615705	-2.069511
25	1	0	4.188810	-2.576643	-2.914998
26	1	0	4.497913	1.277544	-1.024660
27	1	0	5.310919	-0.361937	-2.711184
28	7	0	2.503729	0.967448	0.650206
29	6	0	1.381835	1.909812	0.328903
30	1	0	0.462457	1.324532	0.290098
31	1	0	1.568054	2.334800	-0.657851
32	6	0	1.435687	2.926216	1.483524
33	1	0	0.432961	3.148659	1.844732
34	1	0	1.891849	3.858417	1.145166
35	6	0	2.997658	1.159361	1.824597
36	6	0	1.145783	-1.658119	0.503829
37	6	0	2.329890	2.261104	2.560659
38	1	0	3.067193	2.930027	3.013875
39	1	0	1.762055	1.818600	3.390506
40	1	0	3.803357	0.531685	2.192294
41	1	0	1.065736	-2.750004	0.537093
42	1	0	1.291744	-1.302531	1.530640
43	8	0	-0.050754	-1.094223	-0.046718
44	1	0	-2.879210	-0.676505	-2.206905

1809aaa_model4_PhOCH2Ph_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.538073	0.569175	-0.147932
2	6	0	-3.443083	-0.084901	-0.711292
3	6	0	-2.149775	0.448976	-0.621683
4	6	0	-1.982321	1.681079	0.041139
5	6	0	-3.078426	2.341169	0.604221
6	6	0	-4.353924	1.785692	0.513403
7	1	0	-5.529466	0.135316	-0.231655
8	1	0	-3.593002	-1.024544	-1.236804
9	1	0	-2.913897	3.294237	1.096513
10	1	0	-5.201150	2.304979	0.950970
11	6	0	-0.960334	-0.254407	-1.231374
12	6	0	-0.503567	-1.598121	-0.513752
13	1	0	-0.108358	0.422036	-1.227934
14	6	0	-1.021145	-2.745425	-1.284537
15	7	0	-1.406903	-3.636596	-1.921023
16	6	0	-1.055111	-1.701455	0.851167
17	7	0	-1.484134	-1.800976	1.924884
18	6	0	1.566627	1.792216	0.336473
19	6	0	2.190927	2.973261	-0.092070
20	6	0	2.163915	0.554209	0.028057
21	6	0	3.375428	2.941335	-0.823256
22	1	0	1.729907	3.927480	0.147906
23	6	0	3.359922	0.530623	-0.707579
24	6	0	3.959039	1.711547	-1.139341
25	1	0	3.841140	3.867515	-1.145716
26	1	0	3.821894	-0.425375	-0.937756
27	1	0	4.881481	1.673157	-1.710889
28	7	0	1.587489	-0.671175	0.514120
29	6	0	2.366125	-1.331133	1.592951
30	1	0	2.159790	-0.851860	2.555562
31	1	0	3.444997	-1.241198	1.400362
32	6	0	1.932840	-2.797168	1.546333
33	1	0	1.030784	-2.954365	2.142079
34	1	0	2.709156	-3.464526	1.927964
35	6	0	1.096585	-1.667094	-0.443202
36	6	0	0.232722	1.883566	1.033970
37	6	0	1.650880	-3.019799	0.051475
38	1	0	2.586426	-3.218046	-0.480964
39	1	0	0.982845	-3.861515	-0.145629

40	1	0	-1.160921	-0.507742	-2.275699
41	1	0	1.423773	-1.451431	-1.465953
42	1	0	-0.050515	0.921490	1.462026
43	1	0	0.255943	2.634694	1.831376
44	8	0	-0.755185	2.312607	0.052420

1809aab_model4_PhOCH2Ph_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.755858	1.696120	0.059634
2	6	0	-2.433573	-0.266872	-0.544108
3	6	0	2.245521	-0.589280	-0.267555
4	6	0	1.646161	-1.870264	-0.316973
5	6	0	0.207193	-2.051230	-0.708158
6	1	0	-0.006171	-3.109649	-0.903350
7	1	0	-0.015310	-1.486528	-1.619922
8	6	0	0.642993	1.085389	0.541107
9	1	0	0.379419	0.254320	1.189818
10	6	0	-1.972828	-1.438768	0.080076
11	8	0	-0.631097	-1.593245	0.373029
12	6	0	-1.586882	1.872650	1.267796
13	7	0	-2.219631	2.002565	2.231698
14	6	0	-0.578157	3.044029	-0.528377
15	7	0	-0.464438	4.090068	-1.018818
16	7	0	1.467083	0.580895	-0.577019
17	6	0	2.222264	1.757699	-1.070455
18	1	0	3.128546	1.434409	-1.583451
19	1	0	1.603351	2.271858	-1.810916
20	6	0	1.525850	2.144734	1.249486
21	1	0	0.939428	2.930940	1.732751
22	1	0	2.095649	1.642831	2.036208
23	6	0	2.475330	2.685402	0.147841
24	1	0	2.257512	3.724994	-0.104308
25	1	0	3.516775	2.641758	0.479698
26	6	0	-2.859361	-2.433962	0.491732
27	6	0	-4.229485	-2.279573	0.285545
28	1	0	-2.456341	-3.312636	0.984882
29	1	0	-4.916615	-3.054549	0.611437
30	6	0	-3.815231	-0.135585	-0.739187
31	6	0	-4.709118	-1.126288	-0.334244
32	1	0	-4.194456	0.765056	-1.214868
33	1	0	-5.773895	-0.992614	-0.496923
34	6	0	3.609045	-0.505842	0.057585
35	6	0	4.364167	-1.646828	0.326593
36	1	0	4.093467	0.462221	0.109701
37	1	0	5.416439	-1.543452	0.575075
38	6	0	2.415276	-3.000677	-0.023687
39	6	0	3.768824	-2.904942	0.292684
40	1	0	1.938877	-3.976745	-0.061792
41	1	0	4.347070	-3.798121	0.506773
42	6	0	-1.509445	0.831310	-1.028140
43	1	0	-0.714841	0.451709	-1.675037
44	1	0	-2.107346	1.522126	-1.626198

1901aaa_model4_PhCH2OPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.007242	-1.907417	-1.292360
2	6	0	-3.591253	-0.673406	-0.803987
3	6	0	-2.422931	-0.556448	-0.024127
4	6	0	-1.655265	-1.724829	0.245364
5	6	0	-2.095998	-2.952585	-0.246992
6	6	0	-3.262764	-3.052435	-1.008640
7	1	0	-4.904633	-1.971895	-1.898600
8	1	0	-4.163787	0.210325	-1.055697
9	1	0	-1.517735	-3.846065	-0.032450

10	1	0	-3.580817	-4.019321	-1.385237
11	6	0	-1.956082	0.722944	0.487522
12	6	0	-2.647939	1.880676	0.714736
13	1	0	-0.898902	0.770221	0.727471
14	6	0	-4.058681	2.062911	0.546086
15	7	0	-5.201810	2.252527	0.436585
16	6	0	-1.948465	3.033010	1.204610
17	7	0	-1.389210	3.972980	1.602086
18	6	0	1.833650	-0.790798	0.995117
19	6	0	2.147811	-1.309966	2.249352
20	6	0	2.786428	-0.027849	0.257573
21	6	0	3.393999	-1.056582	2.837002
22	1	0	1.417878	-1.898127	2.792193
23	6	0	4.019272	0.226684	0.887115
24	6	0	4.319393	-0.274467	2.157098
25	1	0	3.617082	-1.461518	3.818918
26	1	0	4.762739	0.822251	0.371768
27	1	0	5.286657	-0.054877	2.599458
28	7	0	2.483384	0.494457	-0.998812
29	6	0	3.420036	1.420004	-1.645710
30	1	0	4.425091	0.979842	-1.763369
31	1	0	3.528174	2.335133	-1.052991
32	6	0	2.793557	1.653690	-3.020119
33	1	0	3.514062	2.039498	-3.745870
34	1	0	1.968164	2.370132	-2.942528
35	6	0	1.740087	-0.280953	-2.025638
36	6	0	2.265882	0.254959	-3.369157
37	1	0	1.491142	0.261537	-4.140528
38	1	0	3.090338	-0.370234	-3.729746
39	1	0	0.663868	-0.117016	-1.923984
40	1	0	1.918365	-1.356099	-1.914914
41	8	0	0.597081	-0.939451	0.401702
42	6	0	-0.404064	-1.691831	1.095038
43	1	0	-0.603484	-1.234947	2.073445
44	1	0	-0.053971	-2.714846	1.270722

1901aab_model4_PhCH2OPh_pyrrolidine_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.453714	-1.144076	1.103058
2	6	0	3.663939	-0.157178	0.522971
3	6	0	2.373907	-0.447548	0.034503
4	6	0	1.872427	-1.774896	0.161829
5	6	0	2.685535	-2.749257	0.740868
6	6	0	3.966953	-2.446748	1.207293
7	1	0	5.439396	-0.893145	1.480533
8	1	0	4.040465	0.857115	0.477803
9	1	0	2.310138	-3.764051	0.830444
10	1	0	4.574255	-3.224143	1.659724
11	6	0	1.528827	0.583903	-0.549780
12	6	0	1.880748	1.761012	-1.150214
13	1	0	0.460464	0.400070	-0.495581
14	6	0	3.217102	2.203418	-1.415265
15	7	0	4.285174	2.593845	-1.663265
16	6	0	0.848595	2.649326	-1.601557
17	7	0	0.014587	3.375526	-1.964557
18	6	0	-1.768994	-1.459622	-0.304368
19	6	0	-2.219155	-2.509226	-1.102205
20	6	0	-2.594066	-0.330997	-0.041427
21	6	0	-3.486119	-2.459086	-1.695822
22	1	0	-1.578796	-3.365552	-1.280164
23	6	0	-3.854140	-0.302732	-0.665500
24	6	0	-4.293558	-1.347056	-1.484174
25	1	0	-3.819433	-3.279788	-2.322949
26	1	0	-4.502330	0.551660	-0.512958
27	1	0	-5.274124	-1.283081	-1.946536
28	7	0	-2.125738	0.728796	0.742317
29	6	0	-2.893519	1.979126	0.798306
30	1	0	-3.933048	1.817655	1.130455
31	1	0	-2.928610	2.450174	-0.189772
32	6	0	-2.142581	2.801491	1.844217

33	1	0	-2.746032	3.620949	2.243001
34	1	0	-1.232691	3.226282	1.405974
35	6	0	-1.462291	0.487915	2.052778
36	6	0	-1.795526	1.734832	2.893479
37	1	0	-0.968372	2.021884	3.548136
38	1	0	-2.669384	1.543354	3.525877
39	1	0	-0.383747	0.372255	1.919622
40	1	0	-1.833483	-0.432538	2.518312
41	8	0	-0.506405	-1.427897	0.252960
42	6	0	0.523032	-2.199622	-0.377967
43	1	0	0.471380	-2.054421	-1.465323
44	1	0	0.378063	-3.266553	-0.177896

1904aaa_model4_PhCH2OPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.075780	-1.940584	-0.580622
2	6	0	3.358564	-0.801991	-0.214983
3	6	0	2.016889	-0.878267	0.189695
4	6	0	1.392583	-2.154590	0.202772
5	6	0	2.125084	-3.285303	-0.172238
6	6	0	3.461878	-3.191043	-0.557409
7	1	0	5.114388	-1.844464	-0.881857
8	1	0	3.861262	0.155702	-0.237851
9	1	0	1.636591	-4.255446	-0.159704
10	1	0	4.012336	-4.082889	-0.839848
11	6	0	1.239423	0.339873	0.606665
12	6	0	1.848555	1.591254	1.038020
13	1	0	0.475012	0.569357	-0.396254
14	6	0	2.980355	2.202504	0.459639
15	7	0	3.915884	2.738452	-0.001604
16	6	0	1.146731	2.378641	1.977330
17	7	0	0.556304	3.022887	2.758960
18	6	0	-2.149729	-1.311733	-0.053901
19	6	0	-3.025830	-2.226093	0.531813
20	6	0	-2.587055	0.003056	-0.352541
21	6	0	-4.342868	-1.867691	0.818694
22	1	0	-2.670070	-3.226551	0.752695
23	6	0	-3.921807	0.339789	-0.067134
24	6	0	-4.789829	-0.583506	0.510606
25	1	0	-5.012067	-2.591853	1.271465
26	1	0	-4.286702	1.333170	-0.295263
27	1	0	-5.813665	-0.291845	0.719540
28	7	0	-1.721021	0.985654	-0.879700
29	6	0	-2.083465	2.425070	-0.819618
30	1	0	-2.449108	2.680486	0.177769
31	1	0	-2.882866	2.617383	-1.543762
32	6	0	-0.786234	3.151735	-1.194944
33	1	0	-0.233897	3.418802	-0.290836
34	1	0	-0.982605	4.065885	-1.757245
35	6	0	-0.484735	0.796350	-1.429157
36	6	0	-0.004225	2.105668	-2.009244
37	1	0	-0.274637	2.133658	-3.072737
38	1	0	1.080334	2.219695	-1.943858
39	1	0	-0.292185	-0.150201	-1.920671
40	1	0	0.435477	0.077906	1.296588
41	6	0	-0.051562	-2.343530	0.594189
42	1	0	-0.300791	-3.408701	0.599265
43	1	0	-0.272003	-1.940098	1.589321
44	8	0	-0.864250	-1.650826	-0.384517

1905aaa_model4_PhCH2OPh_pyrrolidine_CN2_ZW_int_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.795313	3.513402	-0.033364
2	6	0	-3.427544	2.392155	0.507013

3	6	0	-2.787815	1.148129	0.579049
4	6	0	-1.467528	1.044809	0.086643
5	6	0	-0.840711	2.168834	-0.461785
6	6	0	-1.494605	3.400875	-0.521016
7	1	0	-3.317749	4.464821	-0.073718
8	1	0	-4.442272	2.479900	0.887131
9	1	0	0.168937	2.075676	-0.846501
10	1	0	-0.989622	4.261732	-0.949108
11	6	0	-3.537488	-0.043037	1.164954
12	6	0	-3.833865	-1.176539	0.181376
13	1	0	-2.965600	-0.465129	2.000389
14	6	0	-3.186734	-2.404394	0.296357
15	7	0	-2.607259	-3.426047	0.420346
16	6	0	-4.739934	-0.977456	-0.863888
17	7	0	-5.514442	-0.785869	-1.730867
18	6	0	1.468887	-1.171448	0.070609
19	6	0	1.013561	-2.495760	0.014245
20	6	0	2.863791	-0.935618	0.035767
21	6	0	1.928033	-3.545701	-0.073319
22	1	0	-0.047956	-2.715924	0.046775
23	6	0	3.767175	-1.996026	-0.059393
24	6	0	3.302051	-3.306579	-0.109738
25	1	0	1.553564	-4.563722	-0.110462
26	1	0	4.832446	-1.796299	-0.072438
27	1	0	4.006612	-4.127926	-0.173030
28	7	0	3.367285	0.407509	0.067197
29	6	0	4.408283	0.879215	-0.906789
30	1	0	3.940052	0.878070	-1.894358
31	1	0	5.244268	0.181916	-0.912672
32	6	0	4.770421	2.279698	-0.387133
33	1	0	4.911157	2.984841	-1.205992
34	1	0	5.694751	2.238038	0.192209
35	6	0	2.933813	1.368973	0.815577
36	6	0	3.587718	2.669689	0.530264
37	1	0	3.880657	3.176316	1.454016
38	1	0	2.853512	3.321713	0.037164
39	1	0	2.153075	1.191860	1.544096
40	1	0	-4.468794	0.333943	1.606294
41	6	0	-0.761956	-0.290152	0.098970
42	1	0	-1.060032	-0.893707	0.960164
43	1	0	-1.003714	-0.864529	-0.802949
44	8	0	0.664522	-0.083645	0.153731

1909aaa_model4_PhCH2OPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.655227	-0.376001	-0.213631
2	6	0	3.510200	0.180402	-0.784392
3	6	0	2.251809	-0.413636	-0.620606
4	6	0	2.151961	-1.604842	0.130639
5	6	0	3.306417	-2.150738	0.703382
6	6	0	4.552852	-1.546455	0.536986
7	1	0	5.618875	0.103017	-0.356918
8	1	0	3.594370	1.090464	-1.372267
9	1	0	3.225976	-3.065904	1.283731
10	1	0	5.434938	-1.988400	0.989954
11	6	0	1.034558	0.248267	-1.232054
12	6	0	0.475459	1.495095	-0.418438
13	1	0	0.214751	-0.455372	-1.345257
14	6	0	1.135314	2.700922	-0.956829
15	7	0	1.649356	3.635400	-1.416662
16	6	0	0.817235	1.429281	1.015887
17	7	0	1.103732	1.440416	2.140272
18	6	0	-1.459038	-1.698400	0.194833
19	6	0	-1.941415	-2.974038	-0.123889
20	6	0	-2.276615	-0.560139	0.003448
21	6	0	-3.230199	-3.131919	-0.634571
22	1	0	-1.318150	-3.845020	0.045550
23	6	0	-3.564885	-0.749388	-0.514880
24	6	0	-4.046127	-2.019053	-0.835070
25	1	0	-3.591605	-4.128164	-0.870569

26	1	0	-4.194504	0.120547	-0.675136
27	1	0	-5.046732	-2.134719	-1.239313
28	7	0	-1.810182	0.736530	0.377144
29	6	0	-2.652857	1.516852	1.308028
30	1	0	-2.561611	1.120725	2.325199
31	1	0	-3.714604	1.469620	1.027548
32	6	0	-2.134314	2.949469	1.174993
33	1	0	-1.280414	3.116251	1.837402
34	1	0	-2.900122	3.689653	1.418659
35	6	0	-1.128502	1.603919	-0.579252
36	6	0	-1.703712	3.007609	-0.297601
37	1	0	-2.582372	3.141178	-0.937358
38	1	0	-1.011571	3.821167	-0.521712
39	1	0	1.272308	0.617145	-2.233331
40	1	0	-1.316920	1.300514	-1.614709
41	8	0	-0.201812	-1.488647	0.697148
42	6	0	0.851369	-2.366707	0.258990
43	1	0	0.576522	-2.801457	-0.710213
44	1	0	0.966614	-3.191485	0.970445

1909aab_model4_PhCH2OPh_pyrrolidine_CN2_PRODUCT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.670380	1.650671	-0.101154
2	6	0	-2.393876	-0.311893	-0.548522
3	6	0	2.316090	-0.557736	-0.258674
4	6	0	1.547651	-1.742672	-0.321716
5	6	0	0.684852	1.105192	0.534572
6	1	0	0.394374	0.239366	1.127270
7	6	0	-2.109549	-1.560697	0.046847
8	6	0	-1.575250	1.973267	1.023126
9	7	0	-2.262311	2.211008	1.927594
10	6	0	-0.426189	2.917823	-0.825999
11	7	0	-0.258095	3.902573	-1.417211
12	7	0	1.683220	0.702660	-0.473193
13	6	0	2.556290	1.877091	-0.675439
14	1	0	3.492646	1.584546	-1.149576
15	1	0	2.054887	2.564104	-1.360564
16	6	0	1.379873	2.186517	1.427638
17	1	0	0.751202	3.072666	1.547281
18	1	0	1.551616	1.787362	2.429924
19	6	0	2.711374	2.524371	0.712772
20	1	0	2.886953	3.601209	0.647433
21	1	0	3.555091	2.082866	1.252041
22	6	0	-3.170394	-2.368663	0.479834
23	6	0	-4.497774	-1.969513	0.359343
24	1	0	-2.943915	-3.336221	0.921409
25	1	0	-5.295378	-2.619224	0.706432
26	6	0	-3.742228	0.064003	-0.673554
27	6	0	-4.786421	-0.738389	-0.224494
28	1	0	-3.973222	1.017713	-1.140391
29	1	0	-5.813718	-0.406820	-0.339119
30	6	0	3.693200	-0.703458	-0.019736
31	6	0	4.276831	-1.958237	0.155124
32	1	0	4.325271	0.173575	0.048877
33	1	0	5.344387	-2.025000	0.341489
34	6	0	2.130086	-2.995271	-0.135445
35	6	0	3.497945	-3.111818	0.106553
36	1	0	1.504132	-3.878635	-0.214666
37	1	0	3.946431	-4.090725	0.242121
38	6	0	-1.370273	0.660280	-1.119755
39	1	0	-0.561819	0.155089	-1.643014
40	1	0	-1.896232	1.287647	-1.842632
41	6	0	-0.721295	-2.094588	0.329184
42	1	0	-0.391562	-1.785401	1.333874
43	1	0	-0.751679	-3.192260	0.334877
44	8	0	0.212183	-1.627906	-0.640803

251aa_model4_Naft_Pirrolidin_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.623463	2.559078	-0.543038
2	6	0	-3.432328	1.480154	-0.268009
3	6	0	-2.875332	0.185140	-0.083939
4	6	0	-1.460282	0.020989	-0.205209
5	6	0	-0.640926	1.148092	-0.517503
6	6	0	-1.223157	2.395476	-0.664707
7	1	0	-4.745252	-0.827149	0.323288
8	1	0	-3.054270	3.546276	-0.675502
9	1	0	-4.507257	1.606163	-0.176332
10	6	0	-3.669231	-0.947656	0.237838
11	6	0	-0.877305	-1.254081	0.034673
12	1	0	-0.603881	3.252652	-0.908270
13	6	0	-1.680268	-2.330532	0.360001
14	6	0	-3.083509	-2.176453	0.450219
15	1	0	-1.232530	-3.301652	0.548654
16	1	0	-3.696790	-3.036478	0.700279
17	6	0	0.808823	0.967130	-0.741217
18	6	0	1.777653	1.656740	-0.049462
19	1	0	1.123841	0.459259	-1.646126
20	6	0	1.497708	2.429969	1.121398
21	7	0	1.300930	3.067255	2.076640
22	6	0	3.147036	1.589354	-0.455847
23	7	0	4.261313	1.529823	-0.791570
24	7	0	0.548902	-1.343537	-0.068883
25	6	0	1.316058	-1.571202	1.186217
26	1	0	1.720504	-0.610015	1.532243
27	1	0	0.664433	-1.958867	1.975544
28	6	0	2.438366	-2.555967	0.808111
29	6	0	1.091716	-2.217030	-1.135679
30	1	0	0.971471	-1.739531	-2.114339
31	1	0	0.559808	-3.178542	-1.168609
32	6	0	2.548594	-2.419281	-0.719802
33	1	0	2.997845	-3.292498	-1.199140
34	1	0	3.145696	-1.540475	-0.986566
35	1	0	2.143757	-3.577930	1.068966
36	1	0	3.373693	-2.335512	1.328342

253ab_model4_Naft_Pirrolidin_CN2_b3lyp631dp_PCMdmso_TS_2.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.948251	2.244807	-0.867879
2	6	0	-3.532698	1.104223	-0.371089
3	6	0	-2.747438	-0.033939	-0.047575
4	6	0	-1.324561	-0.005409	-0.260526
5	6	0	-0.726803	1.241004	-0.664215
6	6	0	-1.545739	2.307991	-0.998526
7	1	0	-4.435663	-1.170929	0.678711
8	1	0	-3.551912	3.108035	-1.128395
9	1	0	-4.606047	1.055022	-0.213301
10	6	0	-3.362414	-1.183796	0.514571
11	6	0	-0.610482	-1.229603	-0.016550
12	1	0	-1.087086	3.235003	-1.330209
13	6	0	-1.234882	-2.313882	0.577797
14	6	0	-2.614069	-2.285162	0.860519
15	1	0	-0.668649	-3.216677	0.776740
16	1	0	-3.083449	-3.153295	1.311132
17	6	0	0.753978	1.496200	-0.644625
18	6	0	1.440275	1.471798	0.643299
19	1	0	1.034226	2.356003	-1.257875
20	6	0	0.894952	0.941148	1.828778
21	7	0	0.470075	0.516647	2.836125
22	6	0	2.754491	1.981643	0.723554
23	7	0	3.846378	2.404462	0.772286
24	7	0	0.733085	-1.363740	-0.436123
25	6	0	1.759395	-2.155965	0.280556
26	1	0	1.725031	-1.928851	1.348028

27	1	0	1.557157	-3.223860	0.139168
28	6	0	3.063594	-1.731013	-0.412209
29	6	0	1.188684	-0.839671	-1.600405
30	1	0	1.234901	0.573722	-1.334230
31	1	0	0.479650	-0.728856	-2.418750
32	6	0	2.611390	-1.296189	-1.823235
33	1	0	2.593777	-2.142227	-2.522587
34	1	0	3.241166	-0.521735	-2.266504
35	1	0	3.792898	-2.542223	-0.438221
36	1	0	3.510702	-0.885828	0.116838

255ab_model4_Naft_Pirrolidin_CN2_INT_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.273776	-1.674046	-1.135814
2	6	0	3.659554	-0.516407	-0.509573
3	6	0	2.688387	0.413745	-0.052620
4	6	0	1.285295	0.163603	-0.276495
5	6	0	0.901467	-1.108404	-0.834630
6	6	0	1.899737	-1.967502	-1.262878
7	1	0	4.179721	1.716105	0.805748
8	1	0	4.011708	-2.385217	-1.492755
9	1	0	4.709024	-0.293788	-0.342267
10	6	0	3.115267	1.574531	0.644794
11	6	0	0.400541	1.218082	0.132832
12	1	0	1.608750	-2.925731	-1.683226
13	6	0	0.842522	2.320707	0.838667
14	6	0	2.211085	2.492935	1.119555
15	1	0	0.141567	3.093736	1.130328
16	1	0	2.539054	3.369618	1.667001
17	6	0	-0.521748	-1.639990	-0.873226
18	6	0	-1.195617	-1.687615	0.492986
19	1	0	-0.480754	-2.634282	-1.337153
20	6	0	-0.458914	-1.780390	1.679889
21	7	0	0.156138	-1.840178	2.681809
22	6	0	-2.573395	-1.913823	0.558877
23	7	0	-3.740505	-2.075354	0.581812
24	7	0	-0.980556	1.258660	-0.284074
25	6	0	-2.105992	1.618045	0.641196
26	1	0	-2.050968	0.978470	1.519908
27	1	0	-1.973056	2.661033	0.938788
28	6	0	-3.357116	1.407380	-0.229677
29	6	0	-1.368627	1.196513	-1.519701
30	1	0	-1.154869	-1.051468	-1.557184
31	1	0	-0.645892	1.065027	-2.316743
32	6	0	-2.826694	1.430391	-1.683191
33	1	0	-2.955773	2.406193	-2.172095
34	1	0	-3.286888	0.689511	-2.342913
35	1	0	-4.099785	2.185359	-0.051290
36	1	0	-3.804536	0.437004	-0.008934

256aa_model4_Naft_Pirrolidin_CN2_TERMEK1_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.913292	-2.466316	0.021046
2	6	0	3.577391	-1.278595	0.208422
3	6	0	2.901455	-0.032907	0.086227
4	6	0	1.487902	-0.019314	-0.174369
5	6	0	0.846545	-1.269217	-0.475545
6	6	0	1.552880	-2.452426	-0.357899
7	1	0	4.690908	1.156495	0.355009
8	1	0	3.436180	-3.412919	0.115776
9	1	0	4.639289	-1.268974	0.437896
10	6	0	3.620240	1.188211	0.177138
11	6	0	0.806127	1.254295	-0.173312
12	1	0	1.059259	-3.388815	-0.601410

13	6	0	1.563396	2.422187	-0.156256
14	6	0	2.963916	2.383447	0.005047
15	1	0	1.079311	3.387690	-0.221794
16	1	0	3.512841	3.320095	0.033951
17	6	0	-0.534118	-1.316228	-1.090504
18	6	0	-1.702097	-0.963758	-0.113073
19	1	0	-0.719795	-2.303690	-1.517663
20	6	0	-2.937082	-0.813032	-0.907167
21	7	0	-3.889510	-0.696476	-1.560181
22	6	0	-1.920074	-2.054920	0.855954
23	7	0	-2.063116	-2.902441	1.635591
24	7	0	-0.600699	1.301119	-0.166373
25	6	0	-1.322281	0.351617	0.688576
26	1	0	-0.598733	-0.587227	-1.902188
27	1	0	-0.672438	0.000744	1.496435
28	6	0	-2.530075	1.133952	1.238954
29	6	0	-1.283011	2.608728	-0.160400
30	1	0	-1.191476	3.093577	-1.136948
31	1	0	-0.840827	3.276137	0.593875
32	6	0	-2.722320	2.273451	0.225144
33	1	0	-3.242443	3.133358	0.652462
34	1	0	-3.287211	1.931706	-0.646013
35	1	0	-2.267187	1.542573	2.218862
36	1	0	-3.416926	0.508791	1.370598

256ab_model4_Naft_Pirrolidin_CN2_TERMEK1_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.114581	-2.402953	0.268919
2	6	0	3.701751	-1.169804	0.157624
3	6	0	2.920683	-0.002356	-0.057944
4	6	0	1.480942	-0.090587	-0.171884
5	6	0	0.911559	-1.415015	-0.167296
6	6	0	1.722761	-2.511422	0.087729
7	1	0	4.675538	1.259851	-0.049571
8	1	0	3.707687	-3.291500	0.460453
9	1	0	4.778337	-1.055980	0.246535
10	6	0	3.592936	1.245693	-0.130213
11	6	0	0.751432	1.164599	-0.231644
12	1	0	1.273112	-3.499754	0.103784
13	6	0	1.471185	2.355521	-0.321443
14	6	0	2.875665	2.403007	-0.287062
15	1	0	0.935313	3.291838	-0.398826
16	1	0	3.375995	3.363963	-0.359620
17	6	0	-0.481076	-1.794857	-0.633889
18	6	0	-1.710828	-0.985943	-0.132372
19	1	0	-0.645937	-2.844688	-0.385753
20	6	0	-1.766520	-0.961767	1.342377
21	7	0	-1.809085	-0.964220	2.501803
22	6	0	-2.916014	-1.682347	-0.629106
23	7	0	-3.846668	-2.233375	-1.049662
24	7	0	-0.640990	1.266921	-0.039847
25	6	0	-1.216165	2.549775	0.407690
26	1	0	-0.708840	2.886821	1.315945
27	1	0	-1.110273	3.338515	-0.352830
28	6	0	-2.692650	2.227926	0.604149
29	6	0	-1.653304	0.473237	-0.727323
30	1	0	-0.522362	-1.727654	-1.728554
31	1	0	-1.415382	0.328329	-1.788980
32	6	0	-2.962484	1.282586	-0.572448
33	1	0	-3.120873	1.859902	-1.488164
34	1	0	-3.840069	0.647728	-0.434540
35	1	0	-3.318977	3.122443	0.577850
36	1	0	-2.852783	1.723140	1.561019

931aa_model1B_chexene_Me_CN2_b3lyp631dp.log

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-4.078950	-0.905449	0.412425
2	6	0	-3.170291	0.306651	0.193390
3	6	0	-1.705754	-0.048688	-0.028234
4	6	0	-1.297636	-1.376926	-0.117552
5	6	0	-2.305177	-2.485220	-0.362311
6	6	0	-3.734834	-1.992403	-0.601049
7	1	0	-3.944635	-1.300141	1.428755
8	1	0	-3.532623	0.882424	-0.669069
9	1	0	-1.979317	-3.084384	-1.220138
10	1	0	-4.423614	-2.841378	-0.537465
11	6	0	0.433739	-3.129286	-0.370465
12	1	0	0.070399	-3.385598	-1.366746
13	1	0	1.523966	-3.155731	-0.401980
14	1	0	0.090402	-3.894176	0.340363
15	6	0	0.916710	-1.189518	1.023686
16	1	0	0.394766	-0.355404	1.496369
17	1	0	1.079485	-1.941710	1.812115
18	7	0	0.021102	-1.778297	0.016253
19	6	0	-0.754252	0.992912	-0.246129
20	6	0	-0.876753	2.365926	-0.148666
21	1	0	0.212769	0.677592	-0.624276
22	6	0	-1.993147	3.084397	0.382516
23	7	0	-2.871610	3.711073	0.822573
24	6	0	0.213607	3.183996	-0.588617
25	7	0	1.102432	3.844571	-0.950499
26	1	0	-2.283169	-3.171337	0.497805
27	1	0	-3.823268	-1.585907	-1.616544
28	1	0	-5.126504	-0.599334	0.328506
29	1	0	-3.253899	0.983222	1.049240
30	6	0	2.274465	-0.732869	0.510807
31	6	0	3.287425	-0.471976	1.443896
32	6	0	2.545643	-0.540368	-0.847534
33	6	0	4.535134	-0.011768	1.029835
34	1	0	3.094505	-0.625261	2.503394
35	6	0	3.798389	-0.083231	-1.264913
36	1	0	1.775617	-0.752448	-1.583415
37	6	0	4.794824	0.184877	-0.328800
38	1	0	5.306183	0.192117	1.766885
39	1	0	3.989797	0.065635	-2.323296
40	1	0	5.766828	0.544033	-0.652496

931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMacn.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.053971	-0.893069	0.323660
2	6	0	-3.123049	0.318161	0.227073
3	6	0	-1.653380	-0.040196	0.038118
4	6	0	-1.260889	-1.395888	-0.059659
5	6	0	-2.271117	-2.448170	-0.475649
6	6	0	-3.674081	-1.903139	-0.754583
7	1	0	-3.966536	-1.363330	1.312061
8	1	0	-3.446005	0.950346	-0.610759
9	1	0	-1.892848	-2.963638	-1.365814
10	1	0	-4.377165	-2.740810	-0.793811
11	6	0	0.374054	-3.241196	-0.091141
12	1	0	0.071883	-3.527997	-1.097960
13	1	0	1.459542	-3.314095	-0.033742
14	1	0	-0.063727	-3.940881	0.629788
15	6	0	0.924646	-1.192747	1.133271
16	1	0	0.406410	-0.356316	1.605440
17	1	0	1.143611	-1.915758	1.930047
18	7	0	-0.009458	-1.852452	0.207298
19	6	0	-0.706114	0.978726	-0.158143
20	6	0	-0.841738	2.371740	-0.122503
21	1	0	0.285845	0.667085	-0.467092
22	6	0	-1.977159	3.113392	0.310316
23	7	0	-2.865183	3.782908	0.667033
24	6	0	0.266940	3.173438	-0.522071
25	7	0	1.172623	3.834620	-0.848276

26	1	0	-2.317098	-3.212446	0.312080
27	1	0	-3.700216	-1.416975	-1.737713
28	1	0	-5.093000	-0.566131	0.216758
29	1	0	-3.228475	0.935414	1.126063
30	6	0	2.240079	-0.729621	0.524788
31	6	0	3.257872	-0.300934	1.389813
32	6	0	2.472706	-0.707168	-0.854571
33	6	0	4.475583	0.150787	0.885089
34	1	0	3.093275	-0.320072	2.464337
35	6	0	3.696303	-0.257733	-1.361683
36	1	0	1.699407	-1.044735	-1.538246
37	6	0	4.699562	0.173406	-0.495231
38	1	0	5.251842	0.482275	1.568338
39	1	0	3.860297	-0.248353	-2.435076
40	1	0	5.649593	0.522154	-0.888462

931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMdce.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.056426	-0.899499	0.329684
2	6	0	-3.128602	0.312822	0.219410
3	6	0	-1.658403	-0.043639	0.031152
4	6	0	-1.262227	-1.395246	-0.064072
5	6	0	-2.271413	-2.456389	-0.460957
6	6	0	-3.677553	-1.919488	-0.739394
7	1	0	-3.965439	-1.359904	1.322492
8	1	0	-3.454716	0.937187	-0.623046
9	1	0	-1.897427	-2.982936	-1.346423
10	1	0	-4.378294	-2.759682	-0.767459
11	6	0	0.387018	-3.229634	-0.115262
12	1	0	0.079615	-3.515423	-1.120964
13	1	0	1.473553	-3.296004	-0.067086
14	1	0	-0.039841	-3.936516	0.605754
15	6	0	0.927076	-1.188639	1.123058
16	1	0	0.407243	-0.352243	1.593575
17	1	0	1.141442	-1.912660	1.920847
18	7	0	-0.002217	-1.844897	0.190092
19	6	0	-0.712038	0.980338	-0.165179
20	6	0	-0.850649	2.370257	-0.123822
21	1	0	0.279080	0.670985	-0.479525
22	6	0	-1.987603	3.106627	0.317136
23	7	0	-2.877262	3.769498	0.680829
24	6	0	0.253875	3.177876	-0.526813
25	7	0	1.154822	3.843227	-0.856049
26	1	0	-2.310566	-3.210796	0.336965
27	1	0	-3.709164	-1.443467	-1.727340
28	1	0	-5.096499	-0.576033	0.222630
29	1	0	-3.234447	0.938057	1.112566
30	6	0	2.246568	-0.725645	0.523291
31	6	0	3.264194	-0.310733	1.394898
32	6	0	2.482513	-0.689476	-0.855082
33	6	0	4.484830	0.141186	0.897798
34	1	0	3.097034	-0.339894	2.468878
35	6	0	3.708960	-0.240008	-1.354678
36	1	0	1.708823	-1.016189	-1.543620
37	6	0	4.711950	0.177514	-0.481506
38	1	0	5.260679	0.462808	1.586189
39	1	0	3.875170	-0.218751	-2.427547
40	1	0	5.663932	0.527323	-0.868947

931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.054191	-0.891202	0.323180
2	6	0	-3.122476	0.319541	0.227789
3	6	0	-1.653010	-0.039586	0.038740

4	6	0	-1.261339	-1.395771	-0.059432
5	6	0	-2.272117	-2.446925	-0.476714
6	6	0	-3.674589	-1.900679	-0.755733
7	1	0	-3.967355	-1.362279	1.311232
8	1	0	-3.444850	0.952534	-0.609667
9	1	0	-1.893813	-2.961991	-1.367081
10	1	0	-4.378194	-2.737865	-0.795781
11	6	0	0.372045	-3.242285	-0.090032
12	1	0	0.070291	-3.528795	-1.097041
13	1	0	1.457421	-3.316014	-0.031829
14	1	0	-0.066835	-3.941433	0.630697
15	6	0	0.924008	-1.193651	1.133792
16	1	0	0.406069	-0.357254	1.606327
17	1	0	1.143193	-1.916860	1.930266
18	7	0	-0.010626	-1.853173	0.208152
19	6	0	-0.705249	0.978477	-0.157430
20	6	0	-0.839975	2.371838	-0.122080
21	1	0	0.286658	0.666232	-0.465903
22	6	0	-1.974940	3.114406	0.310028
23	7	0	-2.862618	3.784824	0.666046
24	6	0	0.269447	3.172534	-0.521177
25	7	0	1.175897	3.832965	-0.846948
26	1	0	-2.318948	-3.211713	0.310448
27	1	0	-3.700075	-1.413777	-1.738513
28	1	0	-5.092979	-0.563519	0.216167
29	1	0	-3.227624	0.936137	1.127282
30	6	0	2.239190	-0.730577	0.524720
31	6	0	3.257009	-0.301057	1.389332
32	6	0	2.471589	-0.708945	-0.854698
33	6	0	4.474548	0.150639	0.884132
34	1	0	3.092584	-0.319608	2.463893
35	6	0	3.695011	-0.259513	-1.362276
36	1	0	1.698313	-1.047167	-1.538087
37	6	0	4.698313	0.172443	-0.496252
38	1	0	5.250844	0.482694	1.567079
39	1	0	3.858851	-0.250864	-2.435709
40	1	0	5.648228	0.521108	-0.889867

931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMtol.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.064459	-0.918988	0.370766
2	6	0	-3.150599	0.297749	0.207317
3	6	0	-1.681190	-0.051576	0.004186
4	6	0	-1.273517	-1.389460	-0.090461
5	6	0	-2.279216	-2.478121	-0.417091
6	6	0	-3.699936	-1.969096	-0.673727
7	1	0	-3.949439	-1.348241	1.375225
8	1	0	-3.496977	0.897082	-0.645307
9	1	0	-1.927617	-3.035191	-1.292954
10	1	0	-4.391496	-2.817579	-0.657241
11	6	0	0.424340	-3.180581	-0.236944
12	1	0	0.092778	-3.454282	-1.238935
13	1	0	1.513703	-3.223882	-0.226129
14	1	0	0.039223	-3.917031	0.480122
15	6	0	0.929122	-1.182637	1.073849
16	1	0	0.405488	-0.347928	1.543301
17	1	0	1.120688	-1.917946	1.869215
18	7	0	0.017550	-1.812852	0.106246
19	6	0	-0.737141	0.986531	-0.199606
20	6	0	-0.877290	2.367118	-0.132526
21	1	0	0.245644	0.680385	-0.542810
22	6	0	-2.010612	3.088870	0.349454
23	7	0	-2.899324	3.730252	0.748404
24	6	0	0.215467	3.187210	-0.553460
25	7	0	1.105199	3.857344	-0.898512
26	1	0	-2.284101	-3.203296	0.409494
27	1	0	-3.763017	-1.525600	-1.675343
28	1	0	-5.109611	-0.608154	0.276482
29	1	0	-3.248785	0.947638	1.082813
30	6	0	2.266980	-0.720783	0.515756

31	6	0	3.286759	-0.388874	1.419066
32	6	0	2.515733	-0.599886	-0.855208
33	6	0	4.520364	0.068898	0.961661
34	1	0	3.110641	-0.485958	2.487927
35	6	0	3.754883	-0.145225	-1.315560
36	1	0	1.740604	-0.865705	-1.567980
37	6	0	4.758794	0.192370	-0.410030
38	1	0	5.297197	0.327690	1.674972
39	1	0	3.929992	-0.054746	-2.383358
40	1	0	5.720210	0.548436	-0.767113

931aa_model1B_chexene_Me_CN2_b3lyp631dp_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.054147	-0.888822	0.322875
2	6	0	-3.121498	0.321393	0.229366
3	6	0	-1.652344	-0.038682	0.039730
4	6	0	-1.261818	-1.395669	-0.059148
5	6	0	-2.273299	-2.445004	-0.479074
6	6	0	-3.675152	-1.896896	-0.757590
7	1	0	-3.967728	-1.361472	1.310193
8	1	0	-3.443350	0.955769	-0.607239
9	1	0	-1.894940	-2.958521	-1.370299
10	1	0	-4.379500	-2.733368	-0.799109
11	6	0	0.369122	-3.244044	-0.087795
12	1	0	0.067436	-3.530499	-1.094802
13	1	0	1.454369	-3.318811	-0.028933
14	1	0	-0.070932	-3.942186	0.633118
15	6	0	0.923031	-1.194895	1.134752
16	1	0	0.405544	-0.358452	1.607704
17	1	0	1.142561	-1.918272	1.930880
18	7	0	-0.012403	-1.854351	0.209831
19	6	0	-0.703932	0.978076	-0.156377
20	6	0	-0.837463	2.371989	-0.121657
21	1	0	0.287958	0.664997	-0.463993
22	6	0	-1.971917	3.115900	0.308913
23	7	0	-2.859200	3.787625	0.663675
24	6	0	0.273090	3.171216	-0.519922
25	7	0	1.180688	3.830552	-0.844995
26	1	0	-2.321143	-3.211271	0.306539
27	1	0	-3.699928	-1.408413	-1.739601
28	1	0	-5.092684	-0.560221	0.216203
29	1	0	-3.226011	0.936721	1.129844
30	6	0	2.237792	-0.731914	0.524745
31	6	0	3.255684	-0.301175	1.388704
32	6	0	2.469816	-0.711516	-0.854788
33	6	0	4.472921	0.150538	0.882741
34	1	0	3.091577	-0.318949	2.463305
35	6	0	3.692939	-0.262016	-1.363110
36	1	0	1.696613	-1.050764	-1.537721
37	6	0	4.696303	0.171207	-0.497754
38	1	0	5.249306	0.483423	1.565170
39	1	0	3.856506	-0.254451	-2.436584
40	1	0	5.645989	0.519855	-0.891922

933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMacn_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.728933	-2.212335	-2.083878
2	6	0	-1.786023	-0.728856	-1.703403
3	6	0	-0.959709	-0.402379	-0.469417
4	6	0	-0.571250	-1.374343	0.390775
5	6	0	-0.870154	-2.842749	0.196483
6	6	0	-1.962939	-3.088361	-0.851307
7	1	0	-2.475842	-2.419929	-2.857239
8	1	0	-1.444632	-0.102189	-2.536130

9	1	0	0.060249	-3.342638	-0.109326
10	1	0	-2.943820	-2.853578	-0.418847
11	6	0	-0.544274	-1.225666	2.859235
12	1	0	-1.385092	-0.530099	2.969564
13	1	0	-0.925151	-2.244731	2.907890
14	1	0	0.162118	-1.084610	3.677561
15	6	0	0.954725	0.090685	1.485194
16	1	0	0.044214	1.018380	0.781870
17	1	0	1.045660	0.658448	2.411250
18	7	0	0.151292	-1.015064	1.575511
19	6	0	-0.647403	1.048181	-0.254042
20	6	0	-1.747260	1.987248	-0.170041
21	1	0	0.156696	1.405050	-0.908318
22	6	0	-2.976169	1.618694	0.417082
23	7	0	-3.990853	1.292671	0.903288
24	6	0	-1.570735	3.336220	-0.545411
25	7	0	-1.413364	4.451595	-0.866167
26	1	0	-1.150952	-3.304756	1.148078
27	1	0	-1.978836	-4.149307	-1.120373
28	1	0	-0.747533	-2.444854	-2.517032
29	1	0	-2.827536	-0.436644	-1.515759
30	6	0	2.146370	0.138584	0.609336
31	6	0	2.868969	1.343010	0.532696
32	6	0	2.601303	-0.977467	-0.112234
33	6	0	4.014250	1.431541	-0.254695
34	1	0	2.528603	2.209952	1.092727
35	6	0	3.750159	-0.885569	-0.894779
36	1	0	2.073334	-1.920992	-0.037026
37	6	0	4.456827	0.317636	-0.973066
38	1	0	4.562670	2.366850	-0.304619
39	1	0	4.098362	-1.757578	-1.439548
40	1	0	5.351432	0.384368	-1.584330

933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMdce_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.694323	-2.236688	-2.081866
2	6	0	-1.763755	-0.749939	-1.716231
3	6	0	-0.951419	-0.406412	-0.478117
4	6	0	-0.563102	-1.367535	0.393007
5	6	0	-0.850037	-2.839814	0.211596
6	6	0	-1.932626	-3.102599	-0.842795
7	1	0	-2.433691	-2.456762	-2.858980
8	1	0	-1.418786	-0.128983	-2.551822
9	1	0	0.085833	-3.337932	-0.080641
10	1	0	-2.918248	-2.869644	-0.420475
11	6	0	-0.568745	-1.178217	2.857463
12	1	0	-1.411615	-0.481339	2.941212
13	1	0	-0.951109	-2.196271	2.917597
14	1	0	0.123963	-1.022953	3.685070
15	6	0	0.954832	0.109734	1.485122
16	1	0	0.036350	1.038539	0.756417
17	1	0	1.036219	0.691818	2.403023
18	7	0	0.147615	-0.991240	1.581670
19	6	0	-0.654958	1.049918	-0.270433
20	6	0	-1.770034	1.972174	-0.184526
21	1	0	0.135116	1.412739	-0.938588
22	6	0	-2.982967	1.586266	0.424535
23	7	0	-3.980412	1.240863	0.932412
24	6	0	-1.618196	3.320170	-0.574266
25	7	0	-1.477443	4.434005	-0.907352
26	1	0	-1.136370	-3.293237	1.165909
27	1	0	-1.939987	-4.166168	-1.101913
28	1	0	-0.708131	-2.467239	-2.505344
29	1	0	-2.808298	-0.461686	-1.540337
30	6	0	2.148332	0.153386	0.614452
31	6	0	2.873184	1.356786	0.539174
32	6	0	2.604651	-0.963760	-0.105029
33	6	0	4.020966	1.443455	-0.244337
34	1	0	2.531623	2.224873	1.096764
35	6	0	3.756286	-0.873760	-0.883352

36	1	0	2.075255	-1.906588	-0.031326
37	6	0	4.464654	0.328499	-0.960272
38	1	0	4.570327	2.378242	-0.293439
39	1	0	4.105487	-1.746545	-1.426285
40	1	0	5.361285	0.393753	-1.568709

933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMdmso_TS_CH_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.735771	-2.207912	-2.083890
2	6	0	-1.789545	-0.724798	-1.701526
3	6	0	-0.961139	-0.401297	-0.468099
4	6	0	-0.573247	-1.375066	0.390506
5	6	0	-0.874938	-2.842696	0.194362
6	6	0	-1.969728	-3.084953	-0.852075
7	1	0	-2.484158	-2.413112	-2.856465
8	1	0	-1.447864	-0.097824	-2.533902
9	1	0	0.054194	-3.343507	-0.113754
10	1	0	-2.949557	-2.848844	-0.417929
11	6	0	-0.540719	-1.232914	2.859563
12	1	0	-1.380878	-0.537290	2.974365
13	1	0	-0.921809	-2.251964	2.906380
14	1	0	0.168053	-1.094533	3.676261
15	6	0	0.955251	0.086859	1.485347
16	1	0	0.045795	1.015649	0.785307
17	1	0	1.047913	0.652442	2.412571
18	7	0	0.151371	-1.018793	1.574539
19	6	0	-0.645741	1.048273	-0.251644
20	6	0	-1.742965	1.990286	-0.167909
21	1	0	0.160323	1.403778	-0.904215
22	6	0	-2.974109	1.624951	0.416493
23	7	0	-3.991061	1.302090	0.900082
24	6	0	-1.562262	3.339156	-0.541633
25	7	0	-1.401784	4.454500	-0.861006
26	1	0	-1.154963	-3.305788	1.145614
27	1	0	-1.987996	-4.145538	-1.122385
28	1	0	-0.755422	-2.441789	-2.518661
29	1	0	-2.830318	-0.430852	-1.512435
30	6	0	2.146348	0.135100	0.608575
31	6	0	2.870241	1.338845	0.533742
32	6	0	2.599346	-0.980044	-0.115571
33	6	0	4.015004	1.427594	-0.254411
34	1	0	2.531383	2.205042	1.095831
35	6	0	3.747685	-0.887950	-0.898872
36	1	0	2.070329	-1.923104	-0.041841
37	6	0	4.455703	0.314589	-0.975345
38	1	0	4.564508	2.362343	-0.302879
39	1	0	4.094397	-1.759294	-1.445648
40	1	0	5.349903	0.381472	-1.587185

933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMtol_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.512569	-2.404308	-2.041492
2	6	0	-1.645322	-0.897928	-1.789047
3	6	0	-0.906857	-0.438446	-0.544016
4	6	0	-0.513094	-1.320256	0.399974
5	6	0	-0.731558	-2.812107	0.317088
6	6	0	-1.765884	-3.189214	-0.751619
7	1	0	-2.214476	-2.707628	-2.825297
8	1	0	-1.280524	-0.327897	-2.652406
9	1	0	0.231300	-3.295847	0.094943
10	1	0	-2.772621	-2.961601	-0.379680
11	6	0	-0.697409	-0.882592	2.817199
12	1	0	-1.561540	-0.209501	2.745253
13	1	0	-1.063581	-1.899159	2.960334

14	1	0	-0.083621	-0.615828	3.678725
15	6	0	0.936514	0.263265	1.446379
16	1	0	0.009976	1.140908	0.571773
17	1	0	0.958738	0.931274	2.307022
18	7	0	0.125395	-0.825706	1.594431
19	6	0	-0.710287	1.047389	-0.404131
20	6	0	-1.905045	1.862646	-0.271589
21	1	0	-0.016087	1.443365	-1.154304
22	6	0	-2.987744	1.392261	0.501483
23	7	0	-3.849203	0.957482	1.165756
24	6	0	-1.926833	3.191961	-0.746711
25	7	0	-1.921003	4.288680	-1.155327
26	1	0	-1.035795	-3.204895	1.293440
27	1	0	-1.729296	-4.268065	-0.934678
28	1	0	-0.504367	-2.629188	-2.413785
29	1	0	-2.704218	-0.630295	-1.681133
30	6	0	2.158567	0.265989	0.624120
31	6	0	2.887294	1.466442	0.526617
32	6	0	2.642342	-0.877377	-0.035215
33	6	0	4.060782	1.525187	-0.218909
34	1	0	2.524989	2.355901	1.035598
35	6	0	3.820087	-0.815031	-0.775336
36	1	0	2.111219	-1.817538	0.055206
37	6	0	4.529992	0.384384	-0.875236
38	1	0	4.610229	2.458870	-0.285838
39	1	0	4.188771	-1.707548	-1.271536
40	1	0	5.446719	0.427891	-1.455014

933aa_model1B_chexene_Ph_CN2_b3lyp631dp_PCMw_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.978878	-1.974783	-2.107924
2	6	0	-1.911399	-0.516349	-1.643882
3	6	0	-1.008992	-0.325727	-0.435174
4	6	0	-0.673770	-1.377298	0.358337
5	6	0	-1.139822	-2.796023	0.121723
6	6	0	-2.264148	-2.891859	-0.917663
7	1	0	-2.753575	-2.079447	-2.874720
8	1	0	-1.557997	0.133322	-2.453741
9	1	0	-0.273586	-3.389863	-0.203793
10	1	0	-3.215255	-2.598501	-0.455570
11	6	0	-0.389898	-1.649001	2.809372
12	1	0	-1.461087	-1.452890	2.910008
13	1	0	-0.206962	-2.721593	2.906447
14	1	0	0.145653	-1.142965	3.612541
15	6	0	0.980143	-0.093144	1.499528
16	1	0	0.101958	0.932475	0.893189
17	1	0	1.143312	0.368324	2.472955
18	7	0	0.119668	-1.158669	1.515675
19	6	0	-0.563978	1.074997	-0.155246
20	6	0	-1.564282	2.119574	-0.065910
21	1	0	0.296113	1.377316	-0.764612
22	6	0	-2.853745	1.865386	0.446966
23	7	0	-3.924728	1.639440	0.864569
24	6	0	-1.231639	3.456258	-0.373509
25	7	0	-0.944892	4.561185	-0.636099
26	1	0	-1.467750	-3.244700	1.064713
27	1	0	-2.374326	-3.932689	-1.238088
28	1	0	-1.026656	-2.260335	-2.573405
29	1	0	-2.921823	-0.165139	-1.396926
30	6	0	2.142039	-0.022014	0.582822
31	6	0	2.937056	1.137992	0.603586
32	6	0	2.498442	-1.078242	-0.271477
33	6	0	4.059468	1.241024	-0.214754
34	1	0	2.672224	1.958479	1.265102
35	6	0	3.624219	-0.972493	-1.085434
36	1	0	1.910531	-1.988979	-0.278671
37	6	0	4.405213	0.186351	-1.063649
38	1	0	4.665273	2.141229	-0.187276
39	1	0	3.895954	-1.799698	-1.733767
40	1	0	5.281483	0.264070	-1.699670

933aa_model1B_chexene_Ph_CN2_b3lyp631dp_TS_CH_f2.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.413250	-2.481508	-2.011557
2	6	0	-1.571351	-0.967587	-1.827254
3	6	0	-0.881694	-0.444972	-0.580089
4	6	0	-0.495216	-1.281180	0.405676
5	6	0	-0.688421	-2.778758	0.380694
6	6	0	-1.691274	-3.214000	-0.695982
7	1	0	-2.088989	-2.828765	-2.800264
8	1	0	-1.184494	-0.430594	-2.702622
9	1	0	0.285294	-3.261010	0.205212
10	1	0	-2.708847	-2.980598	-0.358794
11	6	0	-0.737696	-0.742857	2.800332
12	1	0	-1.614413	-0.092222	2.681036
13	1	0	-1.088909	-1.759210	2.981798
14	1	0	-0.144632	-0.429630	3.661401
15	6	0	0.941603	0.339175	1.428960
16	1	0	-0.008549	1.213513	0.450805
17	1	0	0.939112	1.048278	2.255832
18	7	0	0.110762	-0.728925	1.594560
19	6	0	-0.743632	1.053917	-0.478135
20	6	0	-1.984300	1.797268	-0.304331
21	1	0	-0.129584	1.463017	-1.288355
22	6	0	-2.964211	1.286743	0.572160
23	7	0	-3.712489	0.802227	1.332617
24	6	0	-2.127970	3.096460	-0.839191
25	7	0	-2.216387	4.166741	-1.302653
26	1	0	-1.013851	-3.133411	1.365156
27	1	0	-1.640326	-4.299461	-0.831605
28	1	0	-0.392471	-2.708927	-2.346953
29	1	0	-2.635698	-0.707333	-1.766126
30	6	0	2.167827	0.323034	0.623489
31	6	0	2.918174	1.512552	0.541258
32	6	0	2.643621	-0.821782	-0.041700
33	6	0	4.099446	1.559874	-0.191053
34	1	0	2.562924	2.404028	1.051882
35	6	0	3.829305	-0.770620	-0.768766
36	1	0	2.097032	-1.754191	0.032928
37	6	0	4.558880	0.417977	-0.852269
38	1	0	4.663017	2.486103	-0.244748
39	1	0	4.189404	-1.664695	-1.268806
40	1	0	5.481731	0.452391	-1.422901

933ba_model1B_chexene_Ph_CN2_b3lyp631dp_PCMdmso_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.867805	-2.650422	0.111740
2	6	0	-2.457885	-1.398550	0.900262
3	6	0	-1.510101	-0.569237	0.051300
4	6	0	-0.391280	-1.241117	-0.481941
5	6	0	-0.321115	-2.753475	-0.397013
6	6	0	-1.649146	-3.532493	-0.198887
7	1	0	-3.611761	-3.229655	0.669372
8	1	0	-3.343822	-0.822345	1.163277
9	1	0	0.202764	-3.146862	-1.268967
10	1	0	-1.498603	-4.239886	0.622568
11	6	0	1.629527	-1.290840	-1.902325
12	1	0	1.078822	-1.878673	-2.636964
13	1	0	2.198218	-0.530338	-2.438378
14	1	0	2.336308	-1.936481	-1.372596
15	6	0	1.174670	0.718259	-0.523711
16	1	0	0.495780	1.056101	0.258645
17	1	0	1.123661	1.441212	-1.344565
18	7	0	0.698110	-0.607170	-0.990742

19	6	0	-1.814010	0.729587	-0.390280
20	6	0	-2.800927	1.639988	0.007878
21	1	0	-1.229096	1.088271	-1.232286
22	6	0	-3.636049	1.530133	1.153822
23	7	0	-4.328566	1.498430	2.094041
24	6	0	-2.973507	2.835843	-0.746172
25	7	0	-3.116021	3.817397	-1.362903
26	1	0	0.353654	-2.959295	0.446821
27	1	0	-1.850635	-4.137402	-1.088044
28	1	0	-3.349260	-2.325265	-0.817756
29	1	0	-1.985344	-1.692127	1.847610
30	6	0	2.590644	0.664631	0.022539
31	6	0	3.610367	1.417485	-0.570297
32	6	0	2.888647	-0.112895	1.151356
33	6	0	4.905798	1.397799	-0.047101
34	1	0	3.389277	2.025179	-1.443965
35	6	0	4.181889	-0.138866	1.671715
36	1	0	2.104521	-0.697636	1.625197
37	6	0	5.194225	0.617745	1.073298
38	1	0	5.686554	1.988631	-0.516656
39	1	0	4.399946	-0.744458	2.546348
40	1	0	6.200693	0.598986	1.480453

951aa_model1C_chexane_Ph_CN2_b3lyp631dp.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.051087	-1.148477	0.720565
2	6	0	-3.473751	0.095654	0.030168
3	6	0	-1.919347	0.073604	0.042065
4	6	0	-1.396142	-1.224934	-0.616993
5	6	0	-1.972409	-2.463741	0.100409
6	6	0	-3.509085	-2.443588	0.101761
7	1	0	-3.794673	-1.118302	1.788166
8	1	0	-3.825151	0.138886	-1.009878
9	1	0	-1.607215	-3.376091	-0.384299
10	1	0	-3.896442	-3.313691	0.643686
11	6	0	0.552623	-2.062509	-1.837798
12	1	0	0.018825	-1.851184	-2.769430
13	1	0	1.615469	-1.875373	-2.006634
14	1	0	0.433474	-3.136341	-1.608478
15	6	0	0.841551	-1.336520	0.457862
16	1	0	0.348172	-0.752843	1.243904
17	1	0	0.849113	-2.383281	0.810759
18	7	0	0.068538	-1.178065	-0.779715
19	6	0	-1.369600	1.268104	-0.671218
20	6	0	-0.991953	2.433419	-0.089379
21	1	0	-1.307647	1.214061	-1.755421
22	6	0	-1.035245	2.619617	1.334929
23	7	0	-1.080916	2.756232	2.489047
24	6	0	-0.528408	3.541337	-0.876880
25	7	0	-0.153424	4.432311	-1.523330
26	1	0	-1.609408	-2.489784	1.136253
27	1	0	-3.874049	-2.533340	-0.931090
28	1	0	-5.145118	-1.124471	0.661634
29	1	0	-3.827540	1.007418	0.522466
30	1	0	-1.605752	0.109542	1.092687
31	1	0	-1.795680	-1.228436	-1.642171
32	6	0	2.278272	-0.857429	0.331697
33	6	0	3.320956	-1.603857	0.891226
34	6	0	2.582893	0.355165	-0.300857
35	6	0	4.639179	-1.147449	0.832213
36	1	0	3.099422	-2.550575	1.378424
37	6	0	3.898816	0.810808	-0.366633
38	1	0	1.780798	0.931374	-0.750427
39	6	0	4.931701	0.062090	0.202459
40	1	0	5.435815	-1.740213	1.272639
41	1	0	4.118030	1.753094	-0.860578
42	1	0	5.956400	0.418449	0.152194

951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMacn.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.042260	-1.124464	0.796971
2	6	0	-3.476984	0.128269	0.112322
3	6	0	-1.921324	0.091046	0.077667
4	6	0	-1.429604	-1.201549	-0.616920
5	6	0	-1.998739	-2.448404	0.089747
6	6	0	-3.534372	-2.411076	0.133843
7	1	0	-3.751051	-1.119361	1.855952
8	1	0	-3.857134	0.192416	-0.915483
9	1	0	-1.657971	-3.352397	-0.426936
10	1	0	-3.914898	-3.288198	0.669089
11	6	0	0.483435	-2.015585	-1.908835
12	1	0	-0.063245	-1.759121	-2.820816
13	1	0	1.547132	-1.843135	-2.090920
14	1	0	0.347191	-3.093535	-1.715493
15	6	0	0.823659	-1.394468	0.408423
16	1	0	0.340212	-0.862400	1.235814
17	1	0	0.836662	-2.459815	0.696507
18	7	0	0.035513	-1.162199	-0.807723
19	6	0	-1.396623	1.284001	-0.650780
20	6	0	-0.955226	2.436855	-0.084353
21	1	0	-1.421717	1.247785	-1.737171
22	6	0	-0.877034	2.616960	1.338036
23	7	0	-0.811297	2.770914	2.489162
24	6	0	-0.538230	3.549414	-0.889369
25	7	0	-0.199631	4.452305	-1.539911
26	1	0	-1.609089	-2.502303	1.114470
27	1	0	-3.929047	-2.473004	-0.889643
28	1	0	-5.137121	-1.086831	0.771316
29	1	0	-3.807216	1.033533	0.631816
30	1	0	-1.571318	0.114682	1.116782
31	1	0	-1.849725	-1.180471	-1.632165
32	6	0	2.258856	-0.904864	0.298975
33	6	0	3.302753	-1.660201	0.847094
34	6	0	2.563378	0.325245	-0.300267
35	6	0	4.619943	-1.195981	0.809452
36	1	0	3.082820	-2.620413	1.307481
37	6	0	3.878480	0.789331	-0.345154
38	1	0	1.760853	0.908056	-0.740428
39	6	0	4.912127	0.031560	0.212557
40	1	0	5.416213	-1.796664	1.239793
41	1	0	4.097297	1.744180	-0.815039
42	1	0	5.935626	0.393324	0.177919

951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMdce.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.042957	-1.129389	0.786647
2	6	0	-3.476622	0.122635	0.101548
3	6	0	-1.920976	0.087889	0.073315
4	6	0	-1.424625	-1.205110	-0.617037
5	6	0	-1.993965	-2.451321	0.090843
6	6	0	-3.529831	-2.416893	0.129256
7	1	0	-3.756575	-1.120977	1.846924
8	1	0	-3.852853	0.184127	-0.927982
9	1	0	-1.649601	-3.356261	-0.421803
10	1	0	-3.910845	-3.293241	0.665389
11	6	0	0.493187	-2.020833	-1.900624
12	1	0	-0.052114	-1.770073	-2.815105
13	1	0	1.556652	-1.846039	-2.081094
14	1	0	0.359557	-3.098418	-1.702938
15	6	0	0.826885	-1.386787	0.414410
16	1	0	0.342183	-0.848291	1.236943
17	1	0	0.839314	-2.450044	0.710628
18	7	0	0.040361	-1.163806	-0.804582
19	6	0	-1.392609	1.280937	-0.653027

20	6	0	-0.961110	2.436254	-0.084626
21	1	0	-1.404455	1.241473	-1.739543
22	6	0	-0.901429	2.619147	1.338484
23	7	0	-0.853064	2.773362	2.490391
24	6	0	-0.537477	3.547453	-0.888352
25	7	0	-0.194263	4.448089	-1.539510
26	1	0	-1.607715	-2.501624	1.117091
27	1	0	-3.920522	-2.482770	-0.895572
28	1	0	-5.137759	-1.093986	0.756370
29	1	0	-3.810625	1.028456	0.617694
30	1	0	-1.576123	0.113023	1.114136
31	1	0	-1.842471	-1.186892	-1.633564
32	6	0	2.262251	-0.898307	0.303029
33	6	0	3.305215	-1.650068	0.857411
34	6	0	2.567498	0.327373	-0.304540
35	6	0	4.622434	-1.186537	0.817680
36	1	0	3.084519	-2.606897	1.324516
37	6	0	3.882650	0.790646	-0.351551
38	1	0	1.765569	0.907351	-0.749467
39	6	0	4.915390	0.036537	0.212394
40	1	0	5.418153	-1.784266	1.253133
41	1	0	4.102030	1.742223	-0.827703
42	1	0	5.938997	0.397850	0.176289

951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.041954	-1.123986	0.798338
2	6	0	-3.476952	0.128831	0.113643
3	6	0	-1.921320	0.091338	0.078001
4	6	0	-1.430136	-1.201147	-0.617106
5	6	0	-1.999178	-2.448107	0.089459
6	6	0	-3.534763	-2.410464	0.134440
7	1	0	-3.750002	-1.119260	1.857118
8	1	0	-3.857712	0.193288	-0.913909
9	1	0	-1.658905	-3.351989	-0.427738
10	1	0	-3.915150	-3.287692	0.669616
11	6	0	0.482442	-2.014717	-1.909995
12	1	0	-0.064539	-1.757670	-2.821624
13	1	0	1.546112	-1.842296	-2.092366
14	1	0	0.346176	-3.092775	-1.717271
15	6	0	0.823253	-1.395373	0.407630
16	1	0	0.339968	-0.864084	1.235629
17	1	0	0.836268	-2.460974	0.694734
18	7	0	0.034961	-1.161978	-0.808188
19	6	0	-1.396962	1.284277	-0.650712
20	6	0	-0.954814	2.436983	-0.084487
21	1	0	-1.422931	1.248205	-1.737081
22	6	0	-0.874926	2.616785	1.337834
23	7	0	-0.807814	2.770948	2.488857
24	6	0	-0.538084	3.549495	-0.889668
25	7	0	-0.199328	4.452436	-1.540068
26	1	0	-1.608975	-2.502441	1.113951
27	1	0	-3.930052	-2.471916	-0.888832
28	1	0	-5.136824	-1.086118	0.773411
29	1	0	-3.806715	1.034011	0.633572
30	1	0	-1.570596	0.114758	1.116890
31	1	0	-1.850497	-1.179731	-1.632224
32	6	0	2.258467	-0.905618	0.298583
33	6	0	3.302455	-1.661475	0.845877
34	6	0	2.562910	0.325129	-0.299406
35	6	0	4.619635	-1.197140	0.808647
36	1	0	3.082599	-2.622193	1.305241
37	6	0	3.877999	0.789343	-0.343875
38	1	0	1.760320	0.908370	-0.738898
39	6	0	4.911728	0.031057	0.213019
40	1	0	5.415968	-1.798234	1.238306
41	1	0	4.096766	1.744688	-0.812792
42	1	0	5.935198	0.392952	0.178724

951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMtol.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.043741	-1.150490	0.752487
2	6	0	-3.475885	0.099659	0.065049
3	6	0	-1.920555	0.075884	0.057748
4	6	0	-1.406333	-1.218275	-0.616770
5	6	0	-1.974955	-2.462688	0.095677
6	6	0	-3.511462	-2.440253	0.114691
7	1	0	-3.772975	-1.130206	1.816713
8	1	0	-3.839474	0.150872	-0.969981
9	1	0	-1.616839	-3.370227	-0.402923
10	1	0	-3.893038	-3.314582	0.653723
11	6	0	0.530054	-2.036852	-1.869985
12	1	0	-0.009602	-1.805985	-2.793279
13	1	0	1.592821	-1.852868	-2.043683
14	1	0	0.406349	-3.113262	-1.657870
15	6	0	0.838598	-1.358826	0.437016
16	1	0	0.349038	-0.798171	1.241850
17	1	0	0.849670	-2.414289	0.761260
18	7	0	0.058524	-1.168492	-0.791786
19	6	0	-1.383556	1.270554	-0.662190
20	6	0	-0.985197	2.433677	-0.087518
21	1	0	-1.354841	1.222091	-1.748048
22	6	0	-0.982322	2.622103	1.336621
23	7	0	-0.985833	2.772074	2.490010
24	6	0	-0.543819	3.543208	-0.884748
25	7	0	-0.187425	4.438853	-1.535472
26	1	0	-1.600724	-2.499737	1.127052
27	1	0	-3.888500	-2.519580	-0.914469
28	1	0	-5.138295	-1.124299	0.707246
29	1	0	-3.823372	1.007191	0.569310
30	1	0	-1.592016	0.107454	1.103766
31	1	0	-1.815065	-1.212279	-1.637790
32	6	0	2.274087	-0.873457	0.318398
33	6	0	3.318115	-1.623121	0.872248
34	6	0	2.577290	0.347937	-0.298134
35	6	0	4.635317	-1.161500	0.823291
36	1	0	3.098352	-2.576624	1.346717
37	6	0	3.892227	0.809143	-0.354103
38	1	0	1.774293	0.926429	-0.743088
39	6	0	4.926270	0.057112	0.209365
40	1	0	5.432471	-1.757164	1.258923
41	1	0	4.110103	1.757930	-0.836253
42	1	0	5.949981	0.417368	0.166718

951aa_model1C_chexane_Ph_CN2_b3lyp631dp_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.041938	-1.123187	0.800050
2	6	0	-3.477112	0.129778	0.115498
3	6	0	-1.921468	0.091986	0.078834
4	6	0	-1.430984	-1.200463	-0.616961
5	6	0	-1.999955	-2.447529	0.089430
6	6	0	-3.535507	-2.409487	0.135248
7	1	0	-3.749298	-1.119007	1.858643
8	1	0	-3.858509	0.194697	-0.911765
9	1	0	-1.660203	-3.351261	-0.428370
10	1	0	-3.915824	-3.286865	0.670237
11	6	0	0.480624	-2.013660	-1.911486
12	1	0	-0.066398	-1.755238	-2.822693
13	1	0	1.544394	-1.841906	-2.093947
14	1	0	0.343514	-3.091755	-1.719742
15	6	0	0.822734	-1.396709	0.406591
16	1	0	0.339593	-0.866604	1.235398
17	1	0	0.835892	-2.462688	0.692192
18	7	0	0.034105	-1.161615	-0.808720

19	6	0	-1.397850	1.284936	-0.650246
20	6	0	-0.953733	2.437102	-0.084370
21	1	0	-1.426430	1.249536	-1.736573
22	6	0	-0.870258	2.616197	1.337802
23	7	0	-0.799865	2.770014	2.488683
24	6	0	-0.538338	3.549923	-0.889774
25	7	0	-0.200632	4.453311	-1.540114
26	1	0	-1.609238	-2.502398	1.113689
27	1	0	-3.931353	-2.470312	-0.887837
28	1	0	-5.136816	-1.085008	0.775791
29	1	0	-3.806306	1.034835	0.636008
30	1	0	-1.569931	0.115232	1.117438
31	1	0	-1.851834	-1.178560	-1.631821
32	6	0	2.257861	-0.906742	0.297828
33	6	0	3.302072	-1.663473	0.843523
34	6	0	2.562121	0.325029	-0.298229
35	6	0	4.619263	-1.199062	0.806622
36	1	0	3.082387	-2.624936	1.301386
37	6	0	3.877216	0.789346	-0.342357
38	1	0	1.759381	0.908979	-0.736492
39	6	0	4.911174	0.030136	0.212921
40	1	0	5.415733	-1.800884	1.234993
41	1	0	4.095817	1.745443	-0.809813
42	1	0	5.934653	0.392004	0.178801

953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_PCMacn_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.165127	-0.872250	0.312174
2	6	0	-3.269352	0.129704	-0.435457
3	6	0	-1.796016	-0.037819	-0.004370
4	6	0	-1.365550	-1.489248	-0.335326
5	6	0	-2.197788	-2.488823	0.480345
6	6	0	-3.689123	-2.324149	0.140275
7	1	0	-4.166375	-0.614614	1.379785
8	1	0	-3.352557	-0.018568	-1.520380
9	1	0	-1.869280	-3.510572	0.260954
10	1	0	-4.290359	-2.994636	0.763701
11	6	0	0.679446	-2.554659	-1.246355
12	1	0	0.666744	-2.093648	-2.243553
13	1	0	1.704878	-2.814976	-0.985788
14	1	0	0.092548	-3.475242	-1.291156
15	6	0	0.800378	-0.669876	0.378048
16	1	0	0.280944	0.474271	-0.209082
17	1	0	0.402182	-0.405509	1.361142
18	7	0	0.101574	-1.696045	-0.216473
19	6	0	-0.860713	0.995824	-0.615670
20	6	0	-0.939749	2.371787	-0.209602
21	1	0	-0.690835	0.866881	-1.687833
22	6	0	-1.444162	2.750920	1.055443
23	7	0	-1.870684	3.059100	2.101624
24	6	0	-0.389319	3.388520	-1.022452
25	7	0	0.059233	4.224115	-1.708812
26	1	0	-2.024102	-2.317452	1.550302
27	1	0	-3.850452	-2.637007	-0.900294
28	1	0	-5.199780	-0.772770	-0.034427
29	1	0	-3.590350	1.155658	-0.229227
30	1	0	-1.769860	0.096484	1.086135
31	1	0	-1.596930	-1.656085	-1.397440
32	6	0	2.276386	-0.529640	0.302081
33	6	0	2.991499	-0.403817	1.505485
34	6	0	2.975064	-0.444003	-0.915744
35	6	0	4.375245	-0.235278	1.494273
36	1	0	2.459726	-0.449094	2.451325
37	6	0	4.356393	-0.265632	-0.923561
38	1	0	2.437683	-0.492934	-1.856527
39	6	0	5.060784	-0.167265	0.279850
40	1	0	4.915160	-0.151508	2.432159
41	1	0	4.882921	-0.195863	-1.870157
42	1	0	6.137459	-0.028774	0.269371

953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_PCMdce_TS_CH_f2.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.165852	-0.864892	0.312097
2	6	0	-3.267353	0.135281	-0.434552
3	6	0	-1.794744	-0.035099	-0.003485
4	6	0	-1.367164	-1.487132	-0.332765
5	6	0	-2.202022	-2.485616	0.481636
6	6	0	-3.692802	-2.317813	0.140430
7	1	0	-4.167535	-0.607293	1.379658
8	1	0	-3.350631	-0.012266	-1.519788
9	1	0	-1.875392	-3.508282	0.263266
10	1	0	-4.295764	-2.987367	0.763178
11	6	0	0.675064	-2.569747	-1.230944
12	1	0	0.665060	-2.121183	-2.234003
13	1	0	1.699269	-2.830829	-0.966484
14	1	0	0.084727	-3.488675	-1.265466
15	6	0	0.802802	-0.675539	0.382119
16	1	0	0.277550	0.482066	-0.212109
17	1	0	0.402546	-0.402383	1.361808
18	7	0	0.099573	-1.696692	-0.212606
19	6	0	-0.855420	0.996007	-0.615505
20	6	0	-0.938475	2.374093	-0.213354
21	1	0	-0.692446	0.866660	-1.688999
22	6	0	-1.437774	2.751115	1.054322
23	7	0	-1.860583	3.051396	2.104241
24	6	0	-0.391855	3.388598	-1.031576
25	7	0	0.054362	4.219120	-1.725398
26	1	0	-2.029000	-2.314505	1.551748
27	1	0	-3.854125	-2.630439	-0.900310
28	1	0	-5.200129	-0.763432	-0.034962
29	1	0	-3.585790	1.161878	-0.228246
30	1	0	-1.768525	0.100113	1.086904
31	1	0	-1.597286	-1.653732	-1.395464
32	6	0	2.276832	-0.534161	0.303470
33	6	0	2.990994	-0.382132	1.504672
34	6	0	2.976765	-0.469495	-0.915283
35	6	0	4.373886	-0.208924	1.491277
36	1	0	2.458580	-0.410142	2.450792
37	6	0	4.357189	-0.286371	-0.925380
38	1	0	2.440731	-0.536844	-1.855666
39	6	0	5.060201	-0.162212	0.276396
40	1	0	4.912584	-0.104364	2.427750
41	1	0	4.884178	-0.231989	-1.872714
42	1	0	6.136288	-0.019531	0.263993

953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_PCMdmso_TS_CH_f2.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.165076	-0.872973	0.312033
2	6	0	-3.269558	0.129126	-0.435725
3	6	0	-1.796162	-0.038070	-0.004518
4	6	0	-1.365365	-1.489460	-0.335558
5	6	0	-2.197400	-2.489116	0.480224
6	6	0	-3.688764	-2.324773	0.140122
7	1	0	-4.166233	-0.615323	1.379646
8	1	0	-3.352667	-0.019326	-1.520603
9	1	0	-1.868671	-3.510783	0.260826
10	1	0	-4.289906	-2.995388	0.763504
11	6	0	0.679944	-2.553099	-1.247864
12	1	0	0.667127	-2.090723	-2.244414
13	1	0	1.705449	-2.813449	-0.987600
14	1	0	0.093311	-3.473781	-1.293868
15	6	0	0.800146	-0.669285	0.377645
16	1	0	0.281288	0.473538	-0.208943
17	1	0	0.402118	-0.405698	1.361023

18	7	0	0.101807	-1.696009	-0.216779
19	6	0	-0.861253	0.995826	-0.615693
20	6	0	-0.939903	2.371559	-0.209129
21	1	0	-0.690782	0.867021	-1.687745
22	6	0	-1.444962	2.750824	1.055612
23	7	0	-1.872003	3.059727	2.101375
24	6	0	-0.388930	3.388536	-1.021299
25	7	0	0.060010	4.224599	-1.706852
26	1	0	-2.023749	-2.317636	1.550167
27	1	0	-3.849956	-2.637595	-0.900467
28	1	0	-5.199777	-0.773686	-0.034487
29	1	0	-3.590859	1.155029	-0.229624
30	1	0	-1.770102	0.096188	1.085991
31	1	0	-1.596804	-1.656357	-1.397612
32	6	0	2.276339	-0.529132	0.301931
33	6	0	2.991612	-0.406271	1.505532
34	6	0	2.974836	-0.441084	-0.915778
35	6	0	4.375447	-0.238278	1.494512
36	1	0	2.459938	-0.453512	2.451335
37	6	0	4.356271	-0.263251	-0.923392
38	1	0	2.437248	-0.487831	-1.856558
39	6	0	5.060862	-0.167836	0.280140
40	1	0	4.915527	-0.156859	2.432514
41	1	0	4.882701	-0.191694	-1.869911
42	1	0	6.137601	-0.029807	0.269835

953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_PCMtol_TS_CH_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.161100	-0.854136	0.327080
2	6	0	-3.263213	0.141037	-0.426258
3	6	0	-1.788947	-0.030981	-0.006311
4	6	0	-1.366331	-1.484220	-0.329567
5	6	0	-2.201028	-2.479510	0.489511
6	6	0	-3.693109	-2.308651	0.155187
7	1	0	-4.156172	-0.594406	1.393996
8	1	0	-3.354794	-0.008059	-1.511169
9	1	0	-1.878676	-3.504889	0.275857
10	1	0	-4.294177	-2.976939	0.781183
11	6	0	0.667332	-2.614404	-1.193449
12	1	0	0.668095	-2.201114	-2.212186
13	1	0	1.686827	-2.880746	-0.916115
14	1	0	0.064265	-3.525945	-1.200446
15	6	0	0.816561	-0.691735	0.382126
16	1	0	0.262573	0.517731	-0.247520
17	1	0	0.404710	-0.383625	1.345284
18	7	0	0.100691	-1.699329	-0.209934
19	6	0	-0.848249	0.998529	-0.628253
20	6	0	-0.950412	2.381389	-0.229992
21	1	0	-0.721558	0.876407	-1.708542
22	6	0	-1.421218	2.739411	1.053882
23	7	0	-1.822063	3.002537	2.122107
24	6	0	-0.431520	3.397264	-1.064512
25	7	0	-0.005110	4.219286	-1.779930
26	1	0	-2.023060	-2.304566	1.558281
27	1	0	-3.860363	-2.622750	-0.884471
28	1	0	-5.197450	-0.751044	-0.013143
29	1	0	-3.575138	1.169435	-0.220762
30	1	0	-1.755522	0.109236	1.083326
31	1	0	-1.596456	-1.655097	-1.392389
32	6	0	2.283019	-0.542550	0.301459
33	6	0	2.983445	-0.289816	1.495303
34	6	0	2.998725	-0.557940	-0.911209
35	6	0	4.362972	-0.098386	1.484012
36	1	0	2.440306	-0.252150	2.435082
37	6	0	4.375900	-0.357240	-0.919310
38	1	0	2.475954	-0.695287	-1.851126
39	6	0	5.063354	-0.134508	0.277073
40	1	0	4.888593	0.085564	2.415651
41	1	0	4.912944	-0.363171	-1.862570
42	1	0	6.137389	0.022646	0.265445

953aa_model1C_chexane_trans_Ph_CN2_b3lyp631dp_TS_CH.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.150122	-0.855685	0.349094
2	6	0	-3.257649	0.136794	-0.412952
3	6	0	-1.779270	-0.031482	-0.010610
4	6	0	-1.357374	-1.484575	-0.327783
5	6	0	-2.189431	-2.479242	0.496352
6	6	0	-3.683859	-2.309995	0.172363
7	1	0	-4.135104	-0.595851	1.415884
8	1	0	-3.361119	-0.013443	-1.497099
9	1	0	-1.869026	-3.506566	0.286806
10	1	0	-4.279451	-2.980619	0.801321
11	6	0	0.665825	-2.664998	-1.149528
12	1	0	0.684580	-2.288012	-2.182738
13	1	0	1.677433	-2.942289	-0.853659
14	1	0	0.044599	-3.564531	-1.132831
15	6	0	0.841873	-0.714394	0.384188
16	1	0	0.245168	0.570416	-0.301176
17	1	0	0.413863	-0.359933	1.322071
18	7	0	0.109980	-1.705637	-0.206226
19	6	0	-0.847995	1.002204	-0.649867
20	6	0	-0.980454	2.389060	-0.249490
21	1	0	-0.769908	0.891455	-1.736943
22	6	0	-1.412423	2.716186	1.055696
23	7	0	-1.783024	2.926640	2.146289
24	6	0	-0.508538	3.414741	-1.099142
25	7	0	-0.118276	4.237180	-1.833767
26	1	0	-2.005774	-2.300480	1.563632
27	1	0	-3.858308	-2.623328	-0.866616
28	1	0	-5.190036	-0.753041	0.019611
29	1	0	-3.564565	1.166399	-0.206845
30	1	0	-1.733795	0.115763	1.077782
31	1	0	-1.586697	-1.660407	-1.390888
32	6	0	2.297221	-0.549972	0.299059
33	6	0	2.979025	-0.169740	1.472733
34	6	0	3.035685	-0.661668	-0.897483
35	6	0	4.352487	0.053073	1.460962
36	1	0	2.422094	-0.055917	2.398343
37	6	0	4.407425	-0.431886	-0.905156
38	1	0	2.532622	-0.891057	-1.829751
39	6	0	5.072904	-0.081642	0.272893
40	1	0	4.859036	0.337651	2.377840
41	1	0	4.958363	-0.512656	-1.837075
42	1	0	6.143298	0.098488	0.260274

953ba_model1C_chexane_trans_Ph_CN2_b3lyp631dp_PCMdmso_TS_CHfix.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.003603	0.855639	-1.906680
2	6	0	2.089239	1.632408	-0.946952
3	6	0	1.120630	0.681473	-0.204348
4	6	0	1.958220	-0.366426	0.560521
5	6	0	2.821208	-1.186761	-0.407998
6	6	0	3.771164	-0.263707	-1.188091
7	1	0	2.391767	0.420497	-2.708182
8	1	0	2.693741	2.179911	-0.211419
9	1	0	3.390554	-1.936510	0.152051
10	1	0	4.351840	-0.849773	-1.908539
11	6	0	1.838477	-1.453738	2.769625
12	1	0	1.931806	-0.541425	3.376777
13	1	0	1.299840	-2.211502	3.341053
14	1	0	2.841250	-1.835484	2.565064
15	6	0	-0.209181	-0.953191	1.600643
16	1	0	-0.308916	0.439588	1.381585

17	1	0	-0.586608	-0.996476	2.624835
18	7	0	1.150186	-1.211140	1.495945
19	6	0	0.168279	1.441565	0.706792
20	6	0	-0.924838	2.176750	0.142532
21	1	0	0.650722	1.946427	1.547315
22	6	0	-1.430437	1.911762	-1.153298
23	7	0	-1.836091	1.713154	-2.232924
24	6	0	-1.593577	3.161402	0.908254
25	7	0	-2.135928	3.976214	1.548876
26	1	0	2.172914	-1.730935	-1.105400
27	1	0	4.494055	0.180342	-0.490145
28	1	0	3.703811	1.547930	-2.387356
29	1	0	1.504635	2.378496	-1.494663
30	1	0	0.519881	0.165697	-0.964214
31	1	0	2.647760	0.196746	1.208853
32	6	0	-1.184318	-1.426516	0.589801
33	6	0	-2.525020	-1.012912	0.704426
34	6	0	-0.818705	-2.275700	-0.466876
35	6	0	-3.471630	-1.423948	-0.229990
36	1	0	-2.819696	-0.369373	1.528970
37	6	0	-1.770381	-2.687315	-1.398479
38	1	0	0.202663	-2.633371	-0.530617
39	6	0	-3.094996	-2.256131	-1.288618
40	1	0	-4.502401	-1.097465	-0.133682
41	1	0	-1.479576	-3.351283	-2.206729
42	1	0	-3.833637	-2.577546	-2.016423
